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Positronium formation as a three-body reaction. I. The second-order positron-electron interaction amplitude

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We derive the exact analytic form for the second-order positron-electron interaction term in the Faddeev three-body approach which is applicable in the nonrelativistic high energy region. Although there is no nonintegrable singularity in the six-dimensional integral form of this amplitude, here the basic difficulty arises from the presence of complex nonintegral exponents in the components included in the integrand. Consequently, three brunch cuts must be handled simultaneously. However, by using an integral representation of the gamma function, these brunch cuts are removed from the integrand. Expanding the radial parts of the initial and final wave functions further reduces the second-order positron-electron interaction term to a one-variable integral in terms of Bessel functions of the third kind. The different final closed expressions are ultimately derived in terms of the generalized hypergeometric functions for different regions of the scattering angle. © *2007 American Institute of Physics.* [DOI: 10.1063/1.2712422]

I. INTRODUCTION

The Coulomb interaction plays an important role in atomic and molecular scattering, where charged particles are involved. The Coulomb potential itself is understood to quite large accuracy. However, its exact incorporation into the quantum mechanical description of atomic and molecular interactions poses difficulties due to its long-range form and the problems associated with that.[1] It is noteworthy that the long-range forms of both the Coulomb and gravitational potentials also create some difficulties in the classical picture as well.[2] The energy shell quantities are involved in describing two-body interactions and the problems associated with them have been investigated in some detail[3] previously. For $n(n>2)$-body interactions, nonetheless, off-shell energy quantities, such as the transition matrix, are important in describing the scattering of the charged particles.[3]

In three-body problems it is convenient to use the integral equation approach rather than successive iterative solutions of the Schrödinger equation,[4] assuming the relevant boundary conditions. In the integral equation approach, the Schrödinger equation governing the three-particle system is converted into appropriate integral equations such as the Lippmann-Schwinger (LS) equation, the distorted wave (DW) integral equation, or the Faddeev-Watson-Lovelace (FWL) equation. Amongst all the integral equation approaches in scattering theory, the LS equation plays a fundamental role. Nonetheless even the LS equation, in its standard form, has ambiguous

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solutions in three- and many-body collisions. The essential difficulty here is that the singular nature of the three-body kernel of the equation invalidates the standard methods of obtaining a solution. Using the language of (perturbation) diagrams (see p. 516 of Ref. 5), the kernel can be thought of as having pathological properties due to disconnected diagrams, where the disconnected diagrams are those in which one of the three particles propagates freely while the other two particles interact via a two-body potential. However, nearly all the useful and efficient scattering formalisms are related to the LS equation either directly or indirectly. For example, among all existing perturbative methods, the continuum distorted wave (CDW) approximation, introduced by Cheshire[6] in 1964, has received considerable attention because it treats the Coulomb interaction properly. This approach can be obtained as a first-order term of the conventional DW formalism of the LS equation,[7] as well as a first-order term of the DW theory of Dodd and Greider,[8] which is a genuine three-body treatment that leads to a connected kernel. We note that the approach of Dodd and Greider[8] is also a kind of appropriate rearrangement of the LS equations.

Another integral equation example is the Faddeev methodology and other related formalisms. In these methods the single three-body LS equation is replaced by a set of three-coupled equations. The kernel in the coupled equations is a 3×3 matrix which, when squared, contains no disconnected diagrams.[9] We note that the Faddeev equations can be derived by combining the homogeneous and inhomogeneous LS equations,[10,11] and we emphasize that the Faddeev and all other similar equations are a suitable rearrangement of the LS equations.

The application of methods based on the Faddeev and other related formalisms to atomic collision problems can become tedious. This is mainly because of a difficulty arising from the complicated nature of the two-body off-shell Coulomb T matrix not having a well-defined on-shell limit. In fact, the off-shell T matrix of a two-body interacting system provides, in principle, all necessary information about the system with the on-shell limit of the off-shell T matrix being related to the scattering amplitude. However, in practice one can show there is no on-shell limit of the Coulomb T matrix, because of the long-range nature of these types of two-body interactions.[12] Even though the long-range nature of the Coulomb potential leads one to expect the propagator of colliding particles to be distorted even in asymptotic form, in our and Alston's theoretical studies the amount of computation is considerably reduced, at the cost of some accuracy of course, by approximating the asymptotic form of the Coulomb Green's function by a free Green's function.

It is worthwhile to note that under some special circumstances the three-coupled equations can be reduced to just two-coupled equations. For example, for scattering of a particle by a two-body bound system, Sitenko[13] has shown that the Faddeev equations governing the different components of the three-body wave function can be reduced to two equations. Also, when the mass of one particle is either much larger or much smaller than the other two, a simplification of the Faddeev-Lovelace coupled integral equations is possible.[8,14] However, this is not followed in this study.

In spite of the limitations in the application of the Faddeev formalism to atomic collisions, as described above, several authors applied that method, in different ways, to solve the three-body collision problems. A separable approach is one of the approximate forms of the FWL formalism, which is based on the Alt-Grassberger-Sandhas[15] (AGS) method. In this approximation the two-particle potential is split into a separable term and a nonseparable remainder. The nonseparable remainder should be small enough for the perturbation series, in powers of this remainder, to converge rapidly. The Faddeev three-particle integral equations now reduce to the effective two-particle equations of a LS type which, after having been expanded in partial waves, become one-dimensional integral equations. Avakov *et al.*[16–19] applied the separable three-body approach to the class of atomic reactions known as electron transfer, while Alt *et al.*[20–22] used the separable approximation for calculation of the electron capture differential cross section for proton-hydrogen scattering. The other method is based on the work of Alston,[23–26] which emphasizes the direct employment of the FWL formalism. Alston has used this method, in a second-order approximation, for calculation of the charge transfer differential cross section of the $1s\rightarrow1s$ transition in the energetic collision of protons with hydrogen and helium atoms.

The FWL formalism has several advantages. First, it is a full quantum mechanical three-body

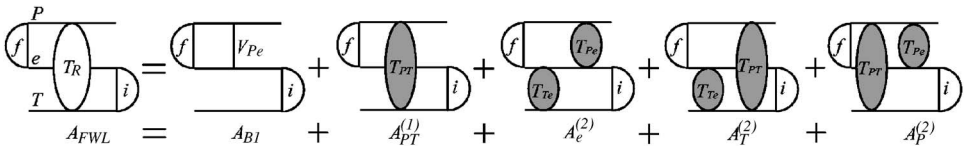

FIG. 1. The Feynman (perturbation) diagrams associated with the five terms in the FWL amplitude for charge exchange. The particles and the interaction potential are denoted by horizontal and vertical lines, respectively. The empty (filled) ellipses represent the transition matrix for the three (two)-body system. However, the open circles are representative of the initial and final bound states. Each diagram indicates one of the terms in Eq. (1).

formalism in which there is no classical assumption. Second, the off-shell two-body T matrices are the principal dynamical ingredients in the FWL approach, rather than the two-body interaction potentials. In other words the whole three-body process can be decomposed in terms of a set of two-body interactions, in which the off-shell T matrices are the essential dynamical elements. Thus, each term in the series obtained by applying the FWL formalisms corresponds to a different physical process such as direct collisions, breakup, and the rearrangement process. Note that each term still contains an infinite-order perturbation series in the treatment of each of the individual scatterings. Moreover, the replacement of potentials with transition operators affords the highest extension in the Born approximations. The third advantage with the FWL formalism is the ability to deal with forward-angle as well as the large-angle projectile scattering within the same formalism, while finally contributions from terms involving the internuclear potentials are also easily assessed in a FWL formalism.

The importance of the Faddeev approach lies in the fact that the kernel of the once iterated Faddeev equations is connected, when the interactions of the three-body system satisfy some reasonable requirements.[27] This kernel is of the Hilbert-Schmidt class, for all but the physical values of energy. As the energy approaches the physical cut, Faddeev[28] has shown that the fifth power of the kernel is compact and without singularities in a certain Banach space of continuous functions. Therefore, the Faddeev equation has unique solutions and the series associated with the FWL formalism are convergent. We should also remember that the convergence of the Born series and some of the perturbative series based on the Born approximation are unknown as yet.[29] On the other hand, the FWL formalism can easily be generalized to higher N-body processes as well as three-body problems.

In this paper, we consider positronium formation in the collision of positrons with atomic hydrogen as being a three-body reaction and we find an exact form for the second-order positron-electron interaction amplitude. The method is applicable to high energy, but nonrelativistic, charge exchange where the speed of the projectile is higher than the speed of the electrons in the target by one to two orders of magnitude. The interaction amplitude under the FWL approach up to the second order,[5,8,9] assuming that the state of the initial channel is $|i\rangle$ and the final channel is $\langle f|$, can be written as

$$A_{\mathrm{FWL}} = \underbrace{\langle f|V_{Pe}|i\rangle}_{A_{B1}} + \underbrace{\langle f|T_{PT}|i\rangle}_{A_{PT}^{(1)}} + \underbrace{\langle f|T_{Te}G_0^{(+)}T_{Pe}|i\rangle}_{A_e^{(2)}} + \underbrace{\langle f|T_{Te}G_0^{(+)}T_{PT}|i\rangle}_{A_T^{(2)}} + \underbrace{\langle f|T_{PT}G_0^{(+)}T_{Pe}|i\rangle}_{A_P^{(2)}}, \quad (1)$$

where V_{xy}, T_{xy}, and $G_0^{(+)}$ are the two-body interaction potential, the two-body transition matrix, and the free Green's operator, respectively. The second-order interaction amplitude therefore includes five terms which are represented using Feynman diagrams in Fig. 1. The first two of these terms are first-order terms, while the other three terms are the second-order terms. Here we will specifically discuss the third term ($A_e^{(2)}$), which we denote as the second-order positron-electron term. In addition we will also find a closed form for it in this paper. Note that discussion on other terms will be presented in future reports.

In Sec. II, we define the notation used in this paper. A closed form for the second-order positron-electron interaction amplitude is subsequently derived in Sec. III. This new form enables us to calculate the second-order positron-electron amplitude quite simply with a personal com-

puter, thereby saving dramatically on the computational cost of the calculations. Concluding remarks and a discussion of our framework are given in Sec. IV. Note that a.u. are used throughout the manuscript.

II. DEFINITIONS

Let us assume that there are three interacting particles, P, T, and e, with masses (charges) of 1 (+1), M_T (Z_T), and 1 (−1), respectively. We shall also distinguish between the effective charge (Z) and the asymptotic charge (Z^a) of the bound system. A free particle P is initially incident on the two-body bound system (T and e) with an incoming velocity $\mathbf{v}_i$ and momentum $\mathbf{K}_i$. This particle then scatters off the bound system and in doing so "picks up" the electron to form a new bound system, positronium, with an outgoing velocity $\mathbf{v}_f$ and momentum $\mathbf{K}_f$, while T remains free. The energy of the initial (final) bound system is $\epsilon_i(\epsilon_f)$. This process is a rearrangement channel and it is usually called electron capture or a charge transfer collision. Let $\mathbf{k}$, $\mathbf{k}'$, and E be the initial channel momentum, the final channel momentum, and the channel energy of a two-body interaction, respectively. In the case of a nonrelativistic high energy projectile, the transition matrix has been simplified previously[23] as

$$T(\mathbf{k},\mathbf{k}';E) = -2\pi Q(Z^a,\mathbf{k};E)Q(Z^a,\mathbf{k}';E)f^C_{\mathbf{k},\mathbf{k}'}(E), \tag{2}$$

where the off-the-shell factor $Q(Z^a,\mathbf{k};E)$ and the Coulomb interaction amplitude $f^C_{\mathbf{k},\mathbf{k}'}(E)$ are

$$Q(Z^a,\mathbf{k};E) = e^{\pi\nu^a/2}\Gamma(1+i\nu^a)[(2\mu E - k^2)/8\mu E]^{-i\nu^a} \tag{3}$$

and

$$f^C_{\mathbf{k},\mathbf{k}'}(E) = 2Ze^{2i\sigma_0}(8\mu E)^{-i\nu}|\mathbf{k}-\mathbf{k}'|^{-2-2i\nu}, \tag{4}$$

respectively, and the Coulomb phase shift for the lth phase shift is defined as

$$\sigma_l = \arg\Gamma(l+1-i\nu), \quad l = 0,1,2,\ldots. \tag{5}$$

The reduced mass of the two interacting particles is denoted by μ. Also, the Sommerfeld parameters are defined as

$$\nu = Z/\mathrm{v} \tag{6}$$

and

$$\nu^a = Z^a/\mathrm{v}. \tag{7}$$

Thus, the final form of the transition matrix will be

$$T(\mathbf{k},\mathbf{k}';E) = -4\pi Ze^{\pi\nu^a}\frac{\Gamma(1+i\nu^a)^2\Gamma(1-i\nu)}{\Gamma(1+i\nu)}(8\mu E)^{-i\nu+2i\nu^a}(2\mu E - k^2)^{-i\nu^a}$$
$$\times(2\mu E - k'^2)^{-i\nu^a}|\mathbf{k}-\mathbf{k}'|^{-2+2i\nu}. \tag{8}$$

To simplify some of the coming formulas, we define the quantities $\tau^a_{jj'}$ and $\tau_{jj'}$ as

$$\tau^a_{jj'} = j\nu^a_P + j'\nu^a_T \tag{9}$$

and

$$\tau_{jj'} = j\nu_P + j'\nu_T \tag{10}$$

for positive and negative values of j and j'. Note that the Sommerfeld parameters associated with the target (ν_T and ν^a_T) and the projectile (ν_P and ν^a_P) correspond to the effective or asymptotic

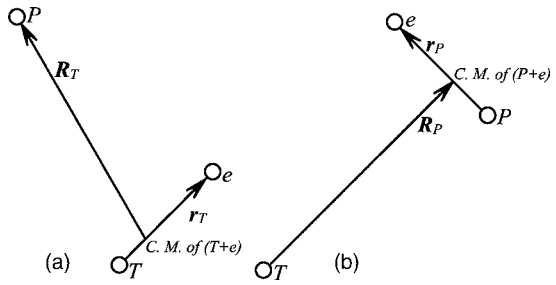

FIG. 2. The Jacobi coordinates for the three particles T, P, and e in (a) the initial and (b) the final channels.

charge and are defined by Eqs. (6) and (7). The wave functions for the initial and final bound system in the momentum representation are

$$\tilde{\phi}_{\text{state}}(\mathbf{k}) \equiv \tilde{\phi}_{nlm}(\mathbf{k}) = R_{nl}(k)Y_{lm}(\hat{\mathbf{k}}), \tag{11}$$

where $R_{nl}(k)(Y_{lm}(\hat{\mathbf{k}}))$ is the radial (angular) part of it. The radial part of the wave function has the simple form

$$R_{nl}(k) = N_{nl}(\alpha_n) \sum_{s=0}^{n-l-1} A_s k^l (k^2 + \alpha_n^2)^{-s-l-2}, \tag{12}$$

where A_s is the expansion coefficient,

$$N_{nl}(\alpha_n) = \sqrt{\frac{2n^{4l+5}(n-l-1)!}{\pi(n+1)!}} l! \alpha_n^{(2l+5)/2} \tag{13}$$

and

$$\alpha_n = \sqrt{-2\mu\varepsilon_n} = \frac{\mu Z}{n}. \tag{14}$$

III. THE POSITRON-ELECTRON SECOND-ORDER AMPLITUDE

As was discussed previously, there are five terms in Eq. (1) and we are interested in the third term, the positron-electron second-order amplitude, namely, $\langle f|T_{Te}G_0^{(+)}T_{Pe}|i\rangle$. Let us now consider a three-body system composed of a bound subsystem of two particles with the relative position vector $\mathbf{r}$ and a free particle with position vector $\mathbf{R}$ with respect to the center of mass of the bound subsystem. The geometry of the scattering channel is presented in Fig. 2 as the Jacobi coordinates. The coordinate and momentum representations of the system (excluding the spin state) in the s channel are defined as:

$$\langle \mathbf{r}, \mathbf{R}|s\rangle = \phi_s(\mathbf{r})e^{i\mathbf{K}_s\cdot\mathbf{R}}$$

and

$$\langle \mathbf{k}, \mathbf{K}|s\rangle = (2\pi)^{9/2}\tilde{\phi}_s(\mathbf{k})\delta(\mathbf{K}-\mathbf{K}_s),$$

where $\phi_s(\mathbf{r})$ $(\tilde{\phi}_s(\mathbf{k}))$ is the wave function of the bound subsystem (its momentum conjugate) and $\mathbf{K}_s$ is the free particle momentum state.

Integrations over the electron momentum in the initial bound subsystem $\mathbf{k}_i$ and the final bound system $\mathbf{k}_f$ are simplified by transformation to the $\mathbf{r}_P$ and $\mathbf{R}_P$ frame and $\mathbf{r}_T$ and $\mathbf{R}_T$ frame, respectively. Substituting the initial and final wave functions, the third term in Eq. (1) would be converted into integral form in the momentum representation as

$$A_e^{(2)} = (2\pi)^{-3} \int \mathrm{d}\mathbf{k}_f \mathrm{d}\mathbf{k}_i \tilde{\phi}_f^*(\mathbf{k}_f) \tilde{\phi}_i(\mathbf{k}_i) \langle \mathbf{k}_f, \mathbf{K}_f | T_{Te} G_0^{(+)} T_{Pe} | \mathbf{k}_i, \mathbf{K}_i \rangle. \tag{15}$$

We will find the inner term,

$$M_1 = \langle \mathbf{k}_f, \mathbf{K}_f | T_{Te} G_0^{(+)} T_{Pe} | \mathbf{k}_i, \mathbf{K}_i \rangle (2\pi)^{-6} \int \mathrm{d}\mathbf{k}_1 \mathrm{d}\mathbf{K}_1 \langle \mathbf{k}_f, \mathbf{K}_f | T_{Te} | \mathbf{k}_1, \mathbf{K}_1 \rangle \langle \mathbf{k}_1, \mathbf{K}_1 | G_0^{(+)} T_{Pe} | \mathbf{k}_i, \mathbf{K}_i \rangle, \tag{16a}$$

by changing variables from the initial and final Jacobi coordinates to the internuclear coordinates described in Fig. 2, and the result will be

$$M_1 = (2\pi)^{-6} \int \mathrm{d}\mathbf{k}_1 \mathrm{d}\mathbf{K}_1 \left\langle \mathbf{k}_f + \frac{1}{2}\mathbf{K}_f, -\mathbf{k}_f + \frac{1}{2}\mathbf{K}_f | T_{Te} | \mathbf{k}_1, \mathbf{K}_1 \right\rangle \times \left\langle \mathbf{k}_1 - \mathbf{K}_1, \mathbf{k}_1 + \mathbf{K}_1 \middle| G_0^{(+)} T_{Pe} \middle| \frac{1}{2}(\mathbf{k}_i - \mathbf{K}_i), \mathbf{k}_i + \mathbf{K}_i \right\rangle. \tag{16b}$$

Implementing some simple algebraic rearrangement of the transition matrices, Eq. (16b) reduces to

$$M_1 = (2\pi)^{-6} \int \mathrm{d}\mathbf{k}_1 \mathrm{d}\mathbf{K}_1 T_{Te}\left(\mathbf{k}_f + \frac{1}{2}\mathbf{K}_f, \mathbf{k}_1; E_f\right) G_0^{(+)}(E_i) T_{Pe}\left(\mathbf{k}_1 - \mathbf{K}_1, \frac{1}{2}(\mathbf{k}_i - \mathbf{K}_i); E_i\right) \times \delta\left(-\mathbf{k}_f + \frac{1}{2}\mathbf{K}_f - \mathbf{K}_1\right) \delta(\mathbf{k}_1 + \mathbf{K}_1 - \mathbf{k}_i - \mathbf{K}_i),$$

leading to the final result as

$$M_1 = T_{Te}\left(\mathbf{k}_f + \frac{1}{2}\mathbf{K}_f, \mathbf{k}_i + \mathbf{k}_f - \mathbf{K}; E_f\right) G_0^{(+)}(E_i) T_{Pe}\left(\mathbf{k}_f + \frac{1}{2}\mathbf{k}_i + \frac{1}{2}\mathbf{J}, \frac{1}{2}(\mathbf{k}_i - \mathbf{K}_i); E_i\right). \tag{16c}$$

Substituting M_1 into Eq. (15), the second-order nuclear-electronic amplitude is

$$A_e^{(2)} = (2\pi)^{-3} \int \mathrm{d}\mathbf{k}_f \mathrm{d}\mathbf{k}_i \tilde{\phi}_f^*(\mathbf{k}_f) \tilde{\phi}_i(\mathbf{k}_i) T_{Te}\left(\mathbf{k}_f + \frac{1}{2}\mathbf{K}_f, \mathbf{k}_i + \mathbf{k}_f - \mathbf{K}; E_f\right) \times G_0^{(+)}(E_i) T_{Pe}\left(\mathbf{k}_f + \frac{1}{2}\mathbf{k}_i + \frac{1}{2}\mathbf{J}, \frac{1}{2}(\mathbf{k}_i - \mathbf{K}_i); E_i\right), \tag{17a}$$

where the free Green's operator is

$$G_0^{(+)}(E_i) = \left(E_i - \left(\mathbf{k}_f + \frac{1}{2}\mathbf{k}_i - \frac{1}{2}\mathbf{J}\right)^2 + i\eta\right)^{-1}, \quad \eta \to 0^+ \tag{17b}$$

or

$$G_0^{(+)}(E_i) = G_0^{(+)}(E_f) = (E_f - (\mathbf{k}_i + \mathbf{k}_f - \mathbf{K})^2/2 + i\eta)^{-1}, \quad \eta \to 0^+. \tag{17c}$$

Here, the momenta $\mathbf{K}[=\mathbf{K}_f/2 - \mathbf{K}_i]$ and $\mathbf{J}[=\mathbf{K}_i - \mathbf{K}_f]$ are the momentum transfer of the projectile and the target, respectively.

We shall now substitute the transition matrices and the free Green's operator into Eq. (17a) to find a more practical expression for the scattering amplitude $A_e^{(2)}$. Incorporating Eq. (2), it is possible to simplify the transition matrices T_{Te} and T_{Pe} as

$$T_{Te}\left(\mathbf{k}_f+\frac{1}{2}\mathbf{K}_f,\mathbf{k}_i+\mathbf{k}_f-\mathbf{K};E_f\right)$$
$$=-2\pi Q\left(Z_T^a,\mathbf{k}_f+\frac{1}{2}\mathbf{K}_f;E_f\right)Q(Z_T^a,\mathbf{k}_i+\mathbf{k}_f-\mathbf{K};E_f)f^C_{\mathbf{k}_f+(1/2)\mathbf{K}_f,\mathbf{k}_i+\mathbf{k}_f-\mathbf{K}}(E_f) \tag{18}$$

and

$$T_{Pe}\left(\mathbf{k}_f+\frac{1}{2}\mathbf{k}_i+\frac{1}{2}\mathbf{J},\frac{1}{2}(\mathbf{k}_i-\mathbf{K}_i);E_i\right)$$
$$=-2\pi Q\left(Z_P^a,\mathbf{k}_f+\frac{1}{2}\mathbf{k}_i+\frac{1}{2}\mathbf{J};E_i\right)Q\left(Z_P^a,\frac{1}{2}(\mathbf{k}_i-\mathbf{K}_i);E_i\right)f^C_{\mathbf{k}_f+(1/2)\mathbf{k}_i+(1/2)\mathbf{J},(1/2)(\mathbf{k}_i-\mathbf{K}_i)}(E_i), \tag{19}$$

respectively. The transition matrices are further simplified by substituting the corresponding relationships for $Q(Z^a,\mathbf{k};E)$ and $f^C_{\mathbf{k},\mathbf{k}'}(E)$, from Eqs. (3) and (4), as

$$T_{Te}\left(\mathbf{k}_f+\frac{1}{2}\mathbf{K}_f,\mathbf{k}_i+\mathbf{k}_f-\mathbf{K};E_f\right)$$
$$=-4\pi Z_T e^{\pi\tau_{01}^a}(8E_f)^{-i\tau_{01}+i\tau_{02}^a}\frac{\Gamma(1+i\tau_{01}^a)^2\Gamma(1-i\tau_{01})}{\Gamma(1+i\tau_{01})}$$
$$\times(2E_f-|\mathbf{k}_f+\mathbf{K}_f/2|^2)^{-i\tau_{01}^a}(2E_f-|\mathbf{k}_i+\mathbf{k}_f-\mathbf{K}|^2)^{-i\tau_{01}^a}|\mathbf{k}_i+\mathbf{J}|^{-2+i\tau_{02}} \tag{20}$$

and

$$T_{Pe}\left(\mathbf{k}_f+\frac{1}{2}\mathbf{k}_i+\frac{1}{2}\mathbf{J},\frac{1}{2}(\mathbf{k}_i-\mathbf{K}_i);E_i\right)$$
$$=-4\pi Z_P e^{\pi\tau_{10}^a}(4E_i)^{-i\tau_{10}+i\tau_{20}^a}\frac{\Gamma(1+i\tau_{10}^a)^2\Gamma(1-i\tau_{10})}{\Gamma(1+i\tau_{10})}$$
$$\times(E_i-|\mathbf{k}_f+\mathbf{k}_i/2+\mathbf{J}/2|^2)^{-i\tau_{10}^a}(E_i-|(\mathbf{k}_i-\mathbf{K}_i)/2|^2)^{-i\tau_{10}^a}|\mathbf{k}_f-\mathbf{K}|^{-2+i\tau_{20}}. \tag{21}$$

There are four arguments that should be found and replaced into Eqs. (20) and (21) as

$$2E_f-|\mathbf{k}_f+\mathbf{K}_f/2|^2=\mathrm{v}_f^2-k_f^2+2\mathbf{k}_f\cdot\mathbf{v}_f+2\varepsilon_f-k_f^2-\mathrm{v}_f^2-2\mathbf{k}_f\cdot\mathbf{v}_f=2(\varepsilon_f-k_f^2), \tag{22}$$

$$E_i-|(\mathbf{k}_i-\mathbf{K}_i)/2|^2=\frac{\mathrm{v}_i^2}{4}-\frac{\mathbf{k}_i\cdot\mathbf{v}_i}{2}-\frac{k_i^2}{4}+\varepsilon_i-\frac{k_i^2}{4}-\frac{v_i^2}{4}+\frac{\mathbf{k}_i\cdot\mathbf{v}_i}{2}=(\varepsilon_i-k_i^2/2), \tag{23}$$

$$E_f-|\mathbf{k}_i+\mathbf{k}_f-\mathbf{K}|^2/2=G_0^{-1}(E_f), \tag{24}$$

and

$$E_i-|\mathbf{k}_f+\mathbf{k}_i/2-\mathbf{J}/2|^2=G_0^{-1}(E_i). \tag{25}$$

Also, we shall make use of the following:

$$E_f \simeq E - \mathrm{v}_f^2/2 \simeq \mathrm{v}_f^2/2 \tag{26}$$

and

$$E_i \simeq E - \mathrm{v}_i^2/4 \simeq \mathrm{v}_i^2/4. \tag{27}$$

Substituting Eqs. (22)–(27) into Eqs. (20) and (21), and in turn substituting these into Eq. (17a), the amplitude is further simplified as follows:

$$A_e^{(2)} = C_1 \int \mathrm{d}\mathbf{k}_f \mathrm{d}\mathbf{k}_i \phi_f^*(\mathbf{k}_f)\phi_i(\mathbf{k}_i)(k_f^2 - \varepsilon_f)^{-i\tau_{01}^a}(k_i^2 - 2\varepsilon_i)^{-i\tau_{10}^a}[G_0^{(+)}]^{1+i\tau_{11}^a}, \tag{28}$$

where

$$C_1 = \left(\frac{2}{\pi}\right) Z_P Z_T e^{\pi\tau_{22}^a} 2^{-i\tau_{02}+i\tau_{12}^a} \mathrm{v}_i^{-i\tau_{20}+i\tau_{40}^a} \mathrm{v}_f^{-i\tau_{02}+4i\tau_{01}^a}$$
$$\times \frac{\Gamma(1+i\tau_{01}^a)^2\Gamma(1-i\tau_{01})\Gamma(1+i\tau_{10}^a)^2\Gamma(1-i\tau_{10})}{\Gamma(1+i\tau_{01})\Gamma(1+i\tau_{10})} J^{-2+i\tau_{02}} K^{-2+i\tau_{20}}.$$

We also have to simplify the free Green's function, Eq. (17b) or (17c), as

$$G_0^{(+)}(E_f) = 2[\kappa + 2\mathbf{k}_i \cdot \mathbf{K} - 2\mathbf{k}_f \cdot \mathbf{J} + i\eta]^{-1}, \tag{29}$$

where

$$\kappa = \mathrm{v}_f^2 - K^2 + 2\varepsilon_f. \tag{30}$$

The amplitude in Eq. (28) now simplifies to the new form

$$A_e^{(2)} = 2^{1+i\tau_{11}^a} C_1 \int \mathrm{d}\mathbf{k}_f \mathrm{d}\mathbf{k}_i \phi_f^*(\mathbf{k}_f)\phi_i(\mathbf{k}_i)(k_f^2 - \varepsilon_f)^{-i\tau_{01}^a}(k_i^2 - 2\varepsilon_i)^{-i\tau_{10}^a}(\kappa + 2\mathbf{k}_i \cdot \mathbf{K} - 2\mathbf{k}_f \cdot \mathbf{J} + i\eta)^{-1-i\tau_{11}^a}. \tag{31}$$

There are three branch cuts in the complex space due to the presence of nonintegral exponents in each factor. To avoid the cut lines, we make use of the identity

$$\beta^{-1-\tau} = \frac{1}{\Gamma(1+\tau)} \int_0^\infty \mathrm{d}y y^\tau e^{-\beta y} \quad \text{for } \mathrm{Re}(\beta) > 0 \text{ and } \mathrm{Re}(\tau) > -1, \tag{32}$$

and we substitute it into Eq. (31). Then the new form for the amplitude will be

$$A_e^{(2)} = C_2 \int_0^\infty \mathrm{d}y y^{i\tau_{11}^a} e^{i\kappa y} \int \mathrm{d}\mathbf{k}_i \phi_i(\mathbf{k}_i) e^{2i\mathbf{k}_i \cdot \mathbf{K} y}(k_i^2 + \alpha_{n_i}^2)^{-i\tau_{10}^a} \int d\mathbf{k}_f \phi_f^*(\mathbf{k}_f) e^{-2i\mathbf{k}_f \cdot \mathbf{J} y}(k_f^2 + \alpha_{n_f}^2)^{-i\tau_{01}^a}, \tag{33}$$

where $C_2 = (2^{1+i\tau_{11}^a} \exp[-i(\pi/2)(1+i\tau_{11}^a)]/\Gamma(1+i\tau_{11}^a))C_1$.

We will further make use of the relation

$$e^{i\mathbf{k}\cdot\mathbf{r}} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y_{lm}^*(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}). \tag{34}$$

Substituting the expansion form of $e^{i\mathbf{k}\cdot\mathbf{r}}$ into the two inner integrals of Eq. (33) and performing the angular integrations over the spherical harmonics, one gets

$$A_e^{(2)} = (4\pi)^2 i^{l_i - l_f} Y_{l_i m_i}(\hat{\mathbf{K}}) Y_{l_f m_f}^*(\hat{\mathbf{J}}) C_2 \int_0^{\infty} \mathrm{d}y y^{i\tau_{11}^a} e^{i\kappa y} \int \mathrm{d}k_i k_i^2 R_{n_i l_i}(k_i)(k_i^2 + \alpha_{n_i}^2)^{-i\tau_{10}^a} j_{l_i}(2Kk_i y)$$
$$\times \int \mathrm{d}k_f k_f^2 R_{n_f l_f}(k_f)(k_f^2 + \alpha_{n_f}^2)^{-i\tau_{01}^a} j_{l_f}(2Jk_f y). \tag{35}$$

Changing now the variable y to a new variable $x = Ky$, the amplitude takes an even simpler form as

$$A_e^{(2)} = C_3 \int_0^{\infty} \mathrm{d}x x^{i\tau_{11}^a} e^{iax} \int \mathrm{d}k_i k_i^2 R_{n_i l_i}(k_i)(k_i^2 + \alpha_{n_i}^2)^{-i\tau_{10}^a} j_{l_i}(k_i x)$$
$$\times \int \mathrm{d}k_f k_f^2 R_{n_f l_f}(k_f)(k_f^2 + \alpha_{n_f}^2)^{-i\tau_{01}^a} j_{l_f}(bk_f x), \tag{36}$$

where $C_3 = (4\pi)^2 (2K)^{-1-i\tau_{11}^a} i^{l_i - l_f} Y_{l_i m_i}(\hat{\mathbf{K}}) Y_{l_f m_f}^*(\hat{\mathbf{J}}) \times C_2$, $a = \kappa/2K$, and $b = J/K$. Replacing the radial part of the initial and final state wave functions, from Eq. (12), into Eq. (36) one arrives at the following result for the amplitude:

$$A_e^{(2)} = C_3 N_{n_i l_i}(\alpha_{n_i}) N_{n_f l_f}(\alpha_{n_f}) \int_0^{\infty} \mathrm{d}x x^{i\tau_{11}^a} e^{iax} \sum_{s_f=0}^{n_f - l_f - 1} \sum_{s=0}^{n_i - l_i - 1} A_{s_f} A_{s_i} \int \mathrm{d}k_i k_i^{2+l_i} (k_i^2 + \alpha_{n_i}^2)^{-2-s_i - l_i - i\tau_{10}^a} j_{l_i}(k_i x)$$
$$\times \int \mathrm{d}k_f k_f^{2+l_f} (k_f^2 + \alpha_{n_f}^2)^{-2-s_f - l_f - i\tau_{01}^a} j_{l_f}(bk_f x)$$
$$= C_3 N_{n_i l_i}(\alpha_{n_i}) N_{n_f l_f}(\alpha_{n_f}) \sum_{s_f=0}^{n_f - l_f - 1} \sum_{s=0}^{n_i - l_i - 1} A_{s_f} A_{s_i} \int_0^{\infty} \mathrm{d}x x^{i\tau_{11}^a} e^{iax} I_{l_i s_i}^{\tau_{10}^a}(\alpha_{n_i}, x) I_{l_f s_f}^{\tau_{01}^a}(\alpha_{n_f}, bx), \tag{37}$$

where

$$I_{ls}^{\tau}(\alpha, x) = \int_0^{\infty} \mathrm{d}k \frac{k^{l+2} j_l(kx)}{(k^2 + \alpha^2)^{l+s+2+i\tau}}. \tag{38}$$

We now use the integral [Eq. (6.565.4) of Ref. 30]

$$\int_0^\infty \mathrm{d}k \frac{k^{\delta+1}\mathrm{J}_\delta(ku)}{(k^2+\alpha^2)^{\zeta+1}} = \frac{u^\zeta \alpha^{\delta-\zeta}}{2^\zeta \Gamma(\zeta+1)} K_{\delta-\zeta}(\alpha u), \qquad -1 < \mathrm{Re}(\delta) < 2\,\mathrm{Re}(\zeta) + \frac{3}{2} \tag{39}$$

and change the Bessel function to a spherical Bessel function [i.e., $j_l(z)=\sqrt{\pi/2z}\mathrm{J}_{l+1/2}(z)$]. Therefore, the integral $I_{ls}^\tau(\alpha,x)$ takes the following form:

$$I_{ls}^\tau(\alpha,x) = \frac{2^{-(l+s+i\tau+3/2)}\pi^{1/2}}{\Gamma(l+s+2+i\tau)} \alpha^{-1/2+s+i\tau} x^{1/2+l+s+i\tau} K_{-1/2-s-i\tau}(\alpha x). \tag{40}$$

We then substitute the result from Eq. (40) into Eq. (36) and arrive at the amplitude as

$$A_e^{(2)} = \sum_{s_f=0}^{n_f-l_f-1} \sum_{s=0}^{n_i-l_i-1} C_4 \int_0^\infty \mathrm{d}x x^{l_i+l_f+s_i+s_f+i\tau_{11}^a+1} e^{iax} K_{-1/2-s_i-i\tau_{10}^a}(\alpha_{n_i} x) K_{-1/2-s_f-i\tau_{01}^a}(\alpha n_f b x) \tag{41}$$

for

$$C_4 = \pi \frac{2^{-(l_i+l_f+s_i+s_f+i\tau_{11}^a+3)} N_{n_i l_i}(\alpha_{n_i}) N_{n_f l_f}(\alpha_{n_f})}{\Gamma(l_i+s_i+2+i\tau_{10}^a)\Gamma(l_f+s_f+2+i\tau_{01}^a)} b^{l_f+s_f+i\tau_{01}^a+1/2} (\alpha_{n_i})^{-s_i-i\tau_{10}^a-1/2} (\alpha_{n_f})^{-s_f-i\tau_{01}^a-1/2} A_{s_i} A_{s_f} C_3.$$

The condition $a=0$ gives rise to the "Thomas peak."[31] We now expand the exponent e^{iax} in Eq. (41) as

$$A_e^{(2)} = \sum_{s_f=0}^{n_f-l_f-1} \sum_{s=0}^{n_i-l_i-1} C_4 \sum_{m=0}^{\infty} \frac{(ia)^m}{m!} \int_0^\infty \mathrm{d}x x^{l_i+l_f+s_i+s_f+m+i\tau_{11}^a+1} K_{-1/2-s_i-i\tau_{10}^a}(\alpha_{n_i} x) K_{-1/2-s_f-i\tau_{01}^a}(\alpha_{n_f} b x), \tag{42}$$

where we denote the inner integral as

$$\mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f}) = C_4 \int_0^\infty \mathrm{d}x x^{1+l_i+l_f+i\tau_{11}^a+s_i+s_f+m} K_{-1/2-s_i-i\tau_{10}^a}(\alpha_{n_i} x) K_{-1/2-s_f-i\tau_{01}^a}(\alpha_{n_f} b x). \tag{43}$$

Let us also make use of the following integral [Eq. (6.576.4) of Ref. 30].

$$\int_0^\infty \mathrm{d}x x^{-\lambda} K_\xi(px) K_\zeta(qx) = \frac{q^\zeta \Gamma((1+\zeta+\xi-\lambda)/2)\Gamma((1+\zeta-\xi-\lambda)/2)\Gamma((1-\zeta+\xi-\lambda)/2)\Gamma((1-\zeta-\xi-\lambda)/2)}{2^{2+\lambda} p^{\zeta-\lambda+1}\Gamma(1-\lambda)} \times {}_2F_1\left(\frac{1+\zeta+\xi-\lambda}{2}, \frac{1+\zeta-\xi-\lambda}{2}; 1-\lambda; 1-q^2/p^2\right), \mathrm{Re}(1-\lambda\pm\xi\pm\zeta) > 0,\ \mathrm{Re}(p+q) > 0. \tag{44}$$

The confluent hypergeometric series ${}_2F_1$ converges for $|1-q^2/p^2|<1$,[32] and Eq. (44) is symmetric with respect to the indices $\xi(p)$ and $\zeta(q)$. Therefore, the convergent form of the integral $\mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f})$ is deduced as

$$\mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f}) = C_5 \frac{2^{-4+m} b^{l_f}}{(\alpha_{n_f})^{1+l_f+2s_f+i\tau^a_{02}} (\alpha_{n_i})^{1+2l_i+l_f+2s_i+i\tau^a_{20}+m}} \times {}_2F_1\left(\frac{1+l_i+l_f+m}{2}, \frac{2+l_i+l_f+2s_i+i\tau^a_{20}+m}{2}; 2+l_i+l_f+s_i+s_f+i\tau^a_{11}+m; 1-\frac{b^2\alpha^2_{n_f}}{\alpha^2_{n_i}} \right) \tag{45}$$

for $0 < b^2\alpha^2_{n_f}/\alpha^2_{n_i} < 2$ or

$$\mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f}) = C_5 \frac{2^{-1+m} (b)^{-1-l_i-m}}{(\alpha_{n_f})^{2+l_i+2l_f+2s_f+i\tau^a_{02}+m} (\alpha_{n_i})^{1+l_i+2s_i+i\tau^a_{20}}} \times {}_2F_1\left(\frac{1+l_i+l_f+m}{2}, \frac{2+l_i+l_f+2s_f+i\tau^a_{02}+m}{2}; 2+l_i+l_f+s_i+s_f+i\tau^a_{11}+m; 1-\frac{\alpha^2_{n_i}}{b^2\alpha^2_{n_f}} \right) \tag{46}$$

for $0 < \alpha^2_{n_i}/b^2\alpha^2_{n_f} < 2$. We are also assuming C_5 to be

$$C_5 = \pi N_{n_i l_i}(\alpha_{n_i}) N_{n_f l_f}(\alpha_{n_f}) A_{s_i} A_{s_f} C_3 \times \frac{\Gamma\left(\frac{(1+l_i+l_f+m)}{2}\right)\Gamma\left(\frac{(2+l_i+l_f+2s_i+i\tau^a_{20}+m)}{2}\right)\Gamma\left(\frac{(2+l_i+l_f+2s_f+i\tau^a_{02}+m)}{2}\right)\Gamma\left(\frac{(3+l_i+l_f+2s_i+2s_f+i\tau^a_{22}+m)}{2}\right)}{\Gamma(l_i+s_i+2+i\tau^a_{10})\Gamma(l_f+s_f+2+i\tau^a_{01})\Gamma(2+l_i+l_f+s_i+s_f+i\tau^a_{11}+m)}.$$

The convergence conditions of the two forms of the integral $\mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f})$ are such that it is always convergent. Therefore, the final form for the positron-electron second-order amplitude is

$$A_e^{(2)} = \sum_{s_f=0}^{n_f-l_f-1} \sum_{s_i=0}^{n_i-l_i-1} \sum_{m=0}^{\infty} \frac{(ia)^m}{m!} \mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f}). \tag{47}$$

We denote the inner summation over m by $\mathfrak{I}_{n_i l_i, n_f l_f, \tau, s_i, s_f}(\alpha_{n_i}, \alpha_{n_f})$ as

$$\mathfrak{I}_{n_i l_i, n_f l_f, \tau, s_i, s_f}(\alpha_{n_i}, \alpha_{n_f}) = \sum_{m=0}^{\infty} \frac{(ia)^m}{m!} \mathfrak{F}_{n_i l_i, n_f l_f, \tau, s_i, s_f, m}(\alpha_{n_i}, \alpha_{n_f}). \tag{48}$$

This summation can be written in terms of the (two-variable) generalized hypergeometric function F_4. To this end, one can use the transformation formulas for confluent hypergeometric series, i.e., Eqs. (9.131.2) and (9.132.1) of Ref. 30, in Eqs. (45) and (46), respectively, and then insert those results into Eq. (47). Expanding the confluent hypergeometric functions, in terms of the powers of their variables, separating the odd and even powers of a, writing the $m!$ in terms of the gamma function, and, finally, doing some mathematical manipulations, the following expressions for $\mathfrak{I}_{n_i l_i, n_f l_f, \tau, s_i, s_f}(\alpha_{n_i}, \alpha_{n_f})$ can be derived:

$$\mathfrak{J}_{n_i l_i, n_f l_f, \tau, s_i, s_f}(\alpha_{n_i}, \alpha_{n_f}) = 2^{-1+l_i+l_f+s_i+s_f+i\tau_{11}} C_4(\alpha_{n_i})^{-2-l_i-l_f-s_i-s_f-i\tau_{11}^a} \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^{1/2+s_f+i\tau_{01}^a}$$
$$\times \left\{ \Gamma\left(-\frac{1}{2} - s_f - i\tau_{01}^a\right)\Gamma\left(\frac{3+l_i+l_f}{2} + s_i + s_f + i\tau_{11}^a\right)\Gamma\left(1 + \frac{l_i+l_f}{2} + s_f + i\tau_{01}^a\right) \right.$$
$$\times F_4\left(\frac{3+l_i+l_f}{2} + s_i + s_f + i\tau_{11}^a, 1 + \frac{l_i+l_f}{2} + s_f + i\tau_{01}^a; \frac{1}{2}, \frac{3}{2}\right.$$
$$\left. + s_f + i\tau_{01}^a; \left(\frac{ia}{\alpha_{n_i}}\right)^2, \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^2\right) + \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^{-1-2s_f-i\tau_{02}^a} \Gamma\left(\frac{1}{2} + s_f + i\tau_{01}^a\right)$$
$$\times \Gamma\left(\frac{2+l_i+l_f}{2} + s_i + i\tau_{10}^a\right)\Gamma\left(\frac{1+l_i+l_f}{2}\right) F_4\left(1 + \frac{l_i+l_f}{2}\right.$$
$$\left. + s_i + i\tau_{10}^a, \frac{1+l_i+l_f}{2}; \frac{1}{2}, \frac{1}{2} - s_f - i\tau_{01}^a; \left(\frac{ia}{\alpha_{n_i}}\right)^2, \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^2\right)$$
$$+ \frac{2ia}{\alpha_{n_i}}\Gamma\left(-\frac{1}{2} - s_f - i\tau_{01}^a\right)\Gamma\left(2 + \frac{l_i+l_f}{2} + s_i + s_f + i\tau_{11}^a\right)$$
$$\times \Gamma\left(\frac{3+l_i+l_f}{2} + s_f + i\tau_{01}^a\right) F_4\left(2 + \frac{l_i+l_f}{2} + s_i + s_f + i\tau_{11}^a, \frac{3+l_i+l_f}{2}\right.$$
$$\left. + s_f + i\tau_{01}^a; \frac{3}{2}, \frac{3}{2} + s_f + i\tau_{01}^a; \left(\frac{ia}{\alpha_{n_i}}\right)^2, \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^2\right) + \frac{2ia}{b\alpha_{n_f}} \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^{-2s_f-i\tau_{02}^a}$$
$$\times \Gamma\left(\frac{1}{2} + s_f + i\tau_{01}^a\right)\Gamma\left(\frac{3+l_i+l_f}{2} + s_i + i\tau_{10}^a\right)\Gamma\left(1 + \frac{l_i+l_f}{2}\right)$$
$$\left. \times F_4\left(\frac{3+l_i+l_f}{2} + s_i + i\tau_{10}^a, 1 + \frac{l_i+l_f}{2}; \frac{3}{2}, \frac{1}{2} - s_f - i\tau_{01}^a; \left(\frac{ia}{\alpha_{n_i}}\right)^2, \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^2\right)\right\} \tag{49}$$

and

$$\mathfrak{J}_{n_i l_i, n_f l_f, \tau, s_i, s_f}(\alpha_{n_i}, \alpha_{n_f}) = (-2) C_4 \left(\frac{-2ia}{\alpha_{n_i}}\right)^{-1-l_i-l_f} \left\{ \left(\frac{-2ia}{\alpha_{n_i}}\right)^{-2-2s_i-2s_f-i\tau_{22}^a} \right.$$
$$\times \Gamma\left(-\frac{1}{2} - s_i - i\tau_{10}^a\right)\Gamma\left(-\frac{1}{2} - s_f - i\tau_{01}^a\right)\Gamma(3 + l_i + l_f + 2s_i + 2s_f + i\tau_{22}^a)$$
$$\times F_4\left(\frac{3+l_i+l_f}{2} + s_i + s_f + i\tau_{11}^a, 2 + \frac{l_i+l_f}{2} + s_i + s_f + i\tau_{11}^a; \frac{3}{2} + s_i + i\tau_{10}^a, \frac{3}{2}\right.$$
$$\left. + s_f + i\tau_{01}^a; \left(\frac{\alpha_{n_i}}{ia}\right)^2, \left(\frac{b\alpha_{n_f}}{ia}\right)^2\right) + \left(\frac{-2ia}{\alpha_{n_i}}\right)^{-1-2s_f} \Gamma\left(\frac{1}{2} + s_i + i\tau_{10}^a\right)$$
$$\times \Gamma\left(-\frac{1}{2} - s_f - i\tau_{01}^a\right)\Gamma(2 + l_i + l_f + 2s_f + i\tau_{02}^a) F_4\left(1 + \frac{l_i+l_f}{2}\right.$$

$$+ s_f + i\tau_{01}^a, \frac{3 + l_i + l_f}{2} + s_f + i\tau_{01}^a; \frac{1}{2} - s_i - i\tau_{10}^a, \frac{3}{2} + s_f + i\tau_{01}^a; \left(\frac{\alpha_{n_i}}{ia}\right)^2, \left(\frac{b\alpha_{n_f}}{ia}\right)^2\Bigg)$$

$$+ \left(\frac{-2ia}{\alpha_{n_i}}\right)^{-1-2s_i-i\tau_{20}^a} \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^{-1-2s_f-i\tau_{02}^a} \Gamma\left(-\frac{1}{2} - s_i - i\tau_{10}^a\right)\Gamma\left(\frac{1}{2} + s_f + i\tau_{01}^a\right)$$

$$\times\Gamma(2 + l_i + l_f + 2s_i + i\tau_{20}^a) F_4\left(1 + \frac{l_i + l_f}{2} + s_i + i\tau_{10}^a, \frac{3 + l_i + l_f}{2} + 2s_i + i\tau_{10}^a; \frac{3}{2}\right.$$

$$\left. + s_i + i\tau_{10}^a, \frac{1}{2} - s_f - i\tau_{01}^a; \left(\frac{\alpha_{n_i}}{ia}\right)^2, \left(\frac{b\alpha_{n_f}}{ia}\right)^2\right)$$

$$+ \left(\frac{b\alpha_{n_f}}{\alpha_{n_i}}\right)^{-1-2s_f-i\tau_{02}^a} \Gamma\left(\frac{1}{2} + s_i + i\tau_{10}^a\right)\Gamma\left(\frac{1}{2} + s_f + i\tau_{01}^a\right)\Gamma(1 + l_i + l_f)$$

$$\times F_4\left(\frac{1 + l_i + l_f}{2}, 1 + \frac{l_i + l_f}{2}; \frac{1}{2} - s_i - i\tau_{10}^a, \frac{1}{2} - s_f - i\tau_{01}^a; \left(\frac{\alpha_{n_i}}{ia}\right)^2, \left(\frac{b\alpha_{n_f}}{ia}\right)^2\right)\Bigg\}. \tag{50}$$

The first expression, Eq. (49), is valid for a range of scattering angles in which $|v^2 - K^2 - \alpha_{n_f}| \leqslant 2K\sqrt{\alpha_{n_i}} - 2J\sqrt{\alpha_{n_f}}$, while the second one, Eq. (50), is applicable in a range of scattering angles which satisfy the inequality $|v^2 - K^2 - \alpha_{n_f}| \geqslant 2K\sqrt{\alpha_{n_i}} + 2J\sqrt{\alpha_{n_f}}$. Therefore, the exact analytic form for the second-order positron-electron interaction term in the Faddeev three-body approach can be written in a closed form as follows:

$$A_e^{(2)} = \sum_{s_f=0}^{n_f - l_f - 1} \sum_{s_i=0}^{n_i - l_i - 1} \Im_{n_i l_i, n_f l_f, \tau, s_i, s_f}(\alpha_{n_i}, \alpha_{n_f}). \tag{51}$$

IV. DISCUSSION AND CONCLUSIONS

Starting from the Faddeev equations, we have obtained a closed form expansion for the second-order positron-electron amplitude. The importance of the second-order positron-electron amplitude lies in the fact that it provides the fully quantum mechanical description of the Thomas peak. This term is simplified to a summation in terms of the confluent hypergeometric function ${}_2F_1$. If one sets $a=0$ in Eq. (41) and performs the procedure leading to Eq. (47), the result will be the same as the term for $m=0$. The final form of the amplitude is expressed as summations of the two-variable generalized hypergeometric functions F_4. Each expression is valid for a definite region of the scattering angles.

The calculations are performed on a personal computer (PC) using MATHEMATICA, and a set of results are plotted in Fig. 3. In Fig. 3, parts (a) and (b), the absolute values and the phase of $A_e^{(2)}$ are, respectively, plotted against the scattering angle, for the collision of 50 keV positrons with atomic hydrogen. Depending on the phase of the other amplitudes in Eq. (1), the constructive or destructive effect of $A_e^{(2)}$ on the other terms can be understood. Note that as claimed in the text, the calculations are valid over all scattering angles. Each data point was calculated in a fraction of a minute, so that the procedure we have outlined here is dramatically cost effective. Finally, we note that in this example, it was assumed that both atomic hydrogen and the final positronium were in a $1s$ state.

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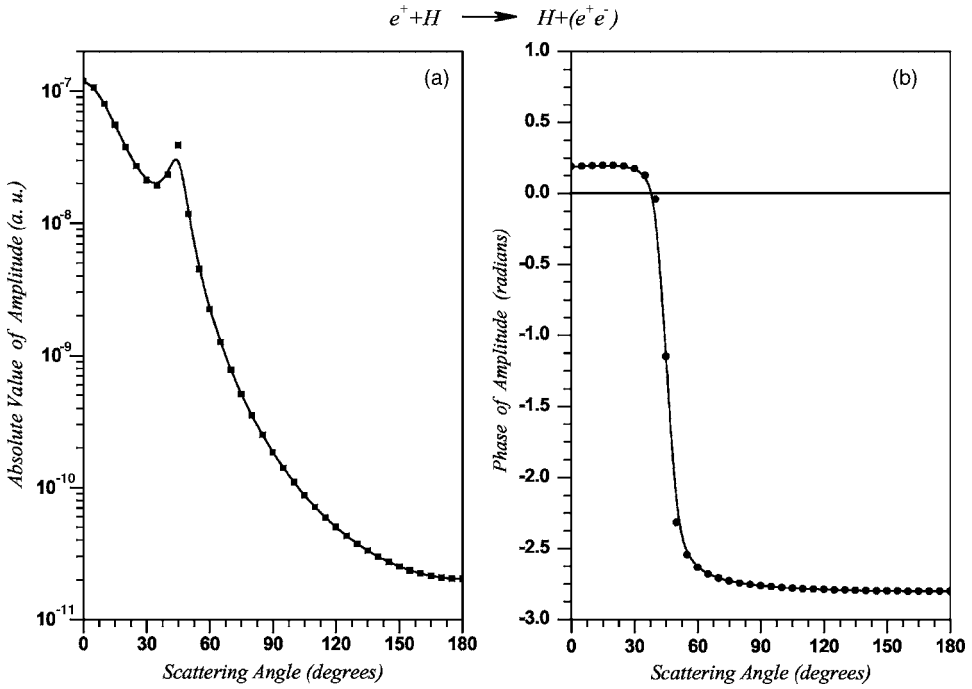

FIG. 3. The calculated values for (a) the absolute value and (b) the phase of $A_e^{(2)}$ are plotted as a function of scattering angle. The data are calculated for the collision of a positron with atomic hydrogen at 50 keV energy, where it is assumed that the final state of positronium was 1*s* as well as the initial state of atomic hydrogen being 1*s*.

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