Zero-range potential for particles interacting via Coulomb potential

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Abstract

The zero-range potential is constructed for a system of two particles interacting via the Coulomb potential. The singular part of the asymptote of the wavefunction at the origin, which is caused by the common effect of the zero-range potential singularity and of the Coulomb potential, is explicitly calculated by using the Lippmann–Schwinger type integral equation. The singular pseudo potential is constructed from the requirement that it enforces the solution to the Coulomb Schrödinger equation to possess the calculated asymptotic behavior at the origin. This pseudo potential is then used for constructing a model of the imaginary absorbing potential for the positron–electron system. This potential allows us to treat the annihilation process in positron–electron collisions on the basis of the non-relativistic Schrödinger equation. The functional form of the pseudo potential constructed in this paper is analogous to the well known Fermi–Breit–Huang pseudo potential. The generalization of the optical theorem in the case of the imaginary absorbing potential in the presence of the Coulomb force is given in terms of the partial wave series.

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1. Introduction

The Dirac delta potential was introduced by Fermi to describe the interaction of neutrons with atomic nucleus [1]. Already at that time it was realized that only perturbative treatment of such a potential is possible [2] due to the strong singularity of the delta function in three dimensions.

One of the possible ways to go beyond the perturbative treatment is the use of the concept of zero-range potentials [2–4]. In this approach, we impose the singular boundary condition

$$\phi(r, k) \sim \frac{\alpha_s}{r} + \beta_s$$

(1)
as \( r \to 0 \). Here, \( \phi(r, k) \) is the solution of the Schrödinger equation

\[
[-\Delta_r + V(r) - k^2]\phi(r, k) = 0, \tag{2}
\]

where \( \Delta \) stands for the Laplacian, bold letters are used for vectors in \( \mathbb{R}^3 \) like \( r \) and \( k \), and \( r = |r| \) and \( k = |k| \). The potential \( V(r) \) here should be of a short-range type, i.e. it should be less singular than \( 1/r^2 \) at the origin and should vanish faster than the Coulomb potential \( 1/r \) as \( r \to \infty \) [5]. The parameters \( \alpha_s \) and \( \beta_s \) are not independent and should be correlated in such a way that the wavefunction \( \phi(r, k) \) is the solution of equation (2) when \( r \to 0 \). As a result, the only independent parameter \( a_s \) of the model can be chosen as \( a_s = -\alpha_s/\beta_s \). In the case of \( V(r) = 0 \), this parameter is the scattering length.

To enforce the boundary condition (1) in an alternative approach [6, 7], an additional term with Dirac delta function \( \delta(r) \) is introduced into the Schrödinger equation

\[
[-\Delta_r + V(r) - k^2]\phi(r, k) + \lambda \delta(r) \beta_s = 0, \tag{3}
\]

where \( \lambda = 4\pi a_s \). Now \( \beta_s \) can be obtained as the limit

\[
\beta_s = \lim_{r \to 0} \frac{d}{dr} \phi(r, k). \tag{4}
\]

This allows us to rewrite (3) as [7]

\[
[-\Delta_r + V(r) + \lambda W_s(r) - k^2]\psi(r, k) = 0, \tag{5}
\]

where

\[
W_s(r) = \delta(r) \frac{d}{dr} r \tag{6}
\]

is a kind of ‘pseudo’ potential. We note that all the above expressions can be derived [5] from the Lippmann–Schwinger equation

\[
\phi(r, k) = \phi_0(r, k) - \lambda \int \, dr' G(r, r', k^2 + i0) W_s(r') \psi(r', k), \tag{7}
\]

where \( \phi_0(r, k) \) is the regular solution to equation (3) with \( \lambda = 0 \) and \( G(r, r', k^2 + i0) \) is the Green function for the Hamiltonian \( -\Delta_r + V(r) \). Here and in what follows by \( i0 \), we mean the limit \( \lim_{\epsilon \to 0} G(r, r', k^2 + i\epsilon) \). The explicit form of \( W \) given in equation (6) is valid only for short-range potentials and it should be modified for long-range potentials like the Coulomb potential [8, 9].

Zero-range potentials are the mathematically correct tools for describing contact interactions. However, in applications the delta function is often used as a potential of contact interaction. A recent example of such an application of the delta function potential is its use in describing the annihilation of positrons in atomic systems [10]. The loss of particles in positron–hydrogen scattering due to the \( e^+e^- \) annihilation can be simulated by an imaginary absorption potential in the positron–electron subsystem. Arguments from perturbative QED [11] suggest a three-dimensional delta function potential [10]. In a series of calculations of positron–hydrogen scattering [10, 12–14], this delta functional potential was smoothed out and the delta function was replaced by a Gaussian with finite width. Thus, the concept of zero-range potentials was not used. Nevertheless, a mathematically sound formulation of how the three-dimensional zero-range potentials in the Coulombic systems can be used is of definite demand. A way for such a formulation was outlined in our paper [15].

In this paper, we continue developing the zero-range potential concept in the presence of Coulomb interaction. We consider the case when the coupling constant \( \lambda \) can be a complex number. It should be noted that the conventional approaches such as [8, 9] cannot be formally applied to this case since the respective operator is not symmetric. In contrast, the approach analogous to equations (3)–(7) can be extended in the case of complex \( \lambda \) and Coulomb...
potential. We give here the detailed derivation of the pseudo potential for the two-body Coulomb Hamiltonian. We show that, as in the short-range case, the Schrödinger equation for this potential can be solved analytically with the help of a Lippmann–Schwinger-type integral equation. We derive from this solution the exact asymptote of the wavefunction at the origin and then the corresponding pseudo potential is constructed. We show that if this potential is treated perturbatively, then it can be taken in the simple form of the delta function as it was used in [10] for the positron–electron case. Finally, we apply the constructed zero-range potential to the description of the positron–electron annihilation by introducing the imaginary absorbing pseudo potential. With this potential, we solve the bound state problem deriving the positronium spectrum as well as the scattering problem calculating the positron–electron wavefunction and the scattering amplitude. The annihilation cross section corresponds to the loss of the flux due to the imaginary absorbing potential. It is calculated by using a generalized optical theorem which we have modified in such a way that it can be applicable to the case of the Coulomb potential.

2. Pseudo potential for Coulomb Hamiltonian

In this section, we construct the zero-range potential and the corresponding pseudo potential for the Coulomb Hamiltonian

\[ H_C = -\Delta_r + n/r. \]  

where

\[ n = \frac{2\mu e^2 Z_1 Z_2}{\hbar^2} \]  

with \( \epsilon = \pm 1 \) for the repulsive and attractive cases, respectively. The Coulomb wavefunction \( \psi_C(r, k) \) satisfies the equation

\[ (H_C - k^2)\psi_C(r, k) = 0. \]  

The explicit form of \( \psi_C(r, k) \) reads [16]

\[ \psi_C(r, k) = \Gamma(1 + i\eta) e^{-\pi\eta/2} e^{i k \cdot r} M(-i\eta, 1; i|kr - k|), \]  

where \( \eta = n/(2k) \), \( \Gamma(z) \) is the gamma function and \( M(a, b; z) \) is the regular Kummer (or confluent hypergeometric) function [17].

Now we construct the zero-range potential and the corresponding pseudo potential along the scheme given by equations (3)–(7). The modified Schrödinger equation reads

\[ [H_C - k^2] \psi(r, k) = -\lambda W(r) \psi(r, k) \]  

and \( W \) is such that

\[ W(r) \psi(r, k) = \delta(r) \beta. \]  

The parameter \( \beta \) should be determined from the solution of the equation (12). This solution, as in the short-range case, can be obtained by solving the Lippmann–Schwinger equation,

\[ \psi(r, k) = \psi_C(r, k) - \lambda \int dr' G_C(r, r', k^2 + i0) W(r') \psi(r', k). \]  

Here \( G_C \) stands for the Coulomb Green function. In view of equation (13), the integration on the right-hand side of equation (14) immediately leads to the representation

\[ \psi(r, k) = \psi_C(r, k) - \lambda G_C(r, 0, k^2 + i0) \beta. \]
From the explicit form of the Coulomb Green function given in [18], one can derive the following representation in terms of the Whittaker function [17]

\[ G_C(r, 0, k^2 + i0) = \frac{1}{4\pi r} \Gamma(1 + i\eta)W_{-i\eta, \frac{1}{2}}(-2ikr). \]  

(16)

This representation is the basis for computing the asymptotic expansion of \( \psi(r, k) \) as \( r \to 0 \).

The Coulomb wavefunction is regular at \( r = 0 \) and can be expanded as

\[ \psi_C(r, k) = \Gamma(1 + i\eta) e^{-\pi\eta/2}[1 + \mathcal{O}(r)]. \]

(17)

The Coulomb Green function \( G_C(r, 0, k^2 + i0) \) is singular as \( r \to 0 \). We will determine the explicit form of this singularity by using representation (16). The Whittaker function can be represented by the irregular Kummer function [17]

\[ W_{\gamma, \mu}(z) = e^{-z^2}z^{\frac{1}{2}+\mu}U(1/2 + \mu - \gamma, 1 + 2\mu, z). \]

(18)

which is valid for \(-\pi < \arg z < \pi\). With \( \gamma = -i\eta \) it results

\[ W_{-i\eta, \frac{1}{2}}(-2ikr) = -2i k r e^{ikr} U(1 + i\eta, 2, -2ikr). \]

(19)

We use the following representation of the irregular Kummer function expansion [17] for integer \( m \)

\[ U(a, m + 1, z) = \frac{(-1)^{m+1}}{m! \Gamma(a-m)} \left[ M(a, m + 1; z) \ln z + \sum_{l=0}^{\infty} \frac{(a)_l}{\Gamma(m+1)_l} \left\{ \psi(a+l) - \psi(1+l) - \psi(1+m+l) \right\} \right] \]

\[ + \frac{(m-1)!}{\Gamma(a)} e^{-z} M(a-m, 1-m; z), \]

(20)

Here, \(-\pi < \arg z < \pi\), \((a)_l = \Gamma(a+l)/\Gamma(a)\) is the Pochhammer symbol, \( \psi(z) = \Gamma'(z)/\Gamma(z) \) is the digamma function and \( M(a, b; z)_m \) is the truncated regular Kummer function defined by the polynomial

\[ M(a, b; z)_m = \sum_{l=0}^{m} \frac{(a)_l}{\Gamma(b)_l} z^l. \]

(21)

The regular Kummer function \( M(a, b; z) \) is given in terms of \( M(a, b; z)_m \) by the limit

\[ M(a, b; z) = \lim_{m \to \infty} M(a, b; z)_m. \]

Using now (20) for the \( U \) factor in (19) with appropriate arguments and keeping the leading terms, we arrive at the following asymptotic representation for that \( U \) factor as \( r \to 0 \)

\[ U(1 + i\eta, 2, -2ikr) = -\frac{1}{2ik} \frac{1}{\Gamma(1 + i\eta)} \left[ 1/r + 2k\eta \log r \right] \]

\[ + \frac{i\eta}{n\Gamma(1 + i\eta)} [4\pi C(k) - ik] + \mathcal{O}(r \log r). \]

(22)

Here \( C(k) \) is given by

\[ C(k) = \frac{ik}{4\pi} + \frac{n}{4\pi} \left[ \log(-2ik) + \psi(1 + i\eta) + 2\gamma_0 - 1 \right], \]

(23)

where \( \gamma_0 \) is the Euler–Mascheroni constant [17]. Substituting (19) and (22) into (16), we obtain the required Coulomb Green function as \( r \to 0 \)

\[ G_C(r, 0, k^2 + i0) = \frac{1}{4\pi} \left[ 1/r + n \log r \right] + C(k) + \mathcal{O}(r \log r). \]

(24)
With these results introduced into (15), we end up with the following asymptotic expansion for the wavefunction as \( r \to 0 \):

\[
\psi(r, k) = -\frac{\lambda}{4\pi} \left[ \frac{1}{r} + n \log r \right] + \psi_{\text{reg}} + O(r \log r),
\]

(25)

where \( \psi_{\text{reg}} = \Gamma(1 + i\eta)e^{-\pi n/2} - \lambda\beta C(k) \) is the regular part, which can be identified as \( \beta = \psi_{\text{reg}} \). The asymptotic expansion of the wavefunction as \( r \to 0 \) now takes the final form

\[
\psi(r, k) = \frac{\alpha}{4\pi} \left[ \frac{1}{r} + n \log r \right] + \beta + O(r \log r),
\]

(26)

and the constants are given by

\[
\alpha = -\frac{\lambda}{4\pi},
\]

(27)

\[
\beta = \Gamma(1 + i\eta)e^{-\pi n/2} \frac{1 + \lambda C(k)}{1 + \lambda C(k)}.
\]

(28)

As in the short-range case, the only independent parameter \( \lambda \) now determines the zero-range potential. Similar to the short-range case, \( \lambda \) is related to the ratio of parameters \( \alpha \) and \( \beta \) by

\[
\lambda = -\frac{\alpha}{\beta}.
\]

At the last stage of our construction, let us represent \( \beta \) in terms of the wavefunction. Introducing a new variable

\[
u = \frac{r}{1 + nr \log r},
\]

it is easy to obtain by direct calculation the following result:

\[
\lim_{r \to 0} \frac{d}{d\nu} u \psi(r, k) = \beta.
\]

(29)

This formula allows us to rewrite the pseudo potential \( W \) in the form

\[
W(r) = \delta(r) \frac{d}{du} u,
\]

and even more explicitly in the final form

\[
W(r) = \delta(r) \frac{(1 + nr \log r)^2}{1 - nr} \frac{d}{dr} \frac{r}{1 + nr \log r}.
\]

(30)

We can see that in the non-Coulomb case, when \( n = 0 \), we recover the short-range result of equation (6).

3. Structure of the Green function

In this section, we construct the Green function for the Hamiltonian \( H_C + \lambda W(r) \). It is the solution of the equation

\[
[H_C + \lambda W - z] G(r, x, z) = \delta(r - x).
\]

(31)

The Green function is symmetric with respect to \( r \) and \( x \) and obeys the boundary condition as \( r \to 0 \)

\[
G(r, x, z) = \frac{A(x, z)}{4\pi} \left[ \frac{1}{r} + n \log r \right] + B(x, z) + O(r \log r).
\]

(32)

Like in equation (13), the action of the quasi-potential on the Green function is given by

\[
W(r)G(r, x, z) = \delta(r)B(x, z).
\]
Thus, we can combine (31) and (32) to obtain
\[ [H_C - z] G(r, x, z) = \delta(r - x) - \lambda \delta(r) B(x, z). \]  
By inverting the operator \( H_C - z \) with the help of the Coulomb Green function, and performing the integration with the delta function, we arrive at the representation
\[ G(r, x, z) = G_C(r, x, z) - \lambda G_C(r, 0, z) B(x, z). \]  
Taking \( r \to 0 \) for a fixed nonzero \( x \) with the use of (24), we arrive at the following asymptotic expression:
\[ G(r, x, z) = -\lambda B(x, z) \frac{1}{4\pi} \left[ \frac{1}{r} + n \log r \right] + G_C(0, x, z) - \lambda B(x, z) C(\sqrt{z}) + \mathcal{O}(r \log r). \]  
Comparing this asymptotic formula with the definition (32), we find the expressions for \( A(x, z) \) and \( B(x, z) \):
\[ A(x, z) = G_C(0, x, z) \frac{-\lambda}{1 + \lambda C(\sqrt{z})}, \]
\[ B(x, z) = G_C(0, x, z) \frac{1}{1 + \lambda C(\sqrt{z})}. \]  
By substituting \( B(x, z) \) into (34), we obtain the final representation for the Green function in the form
\[ G(r, x, z) = G_C(r, x, z) - \lambda G_C(r, 0, z) \frac{1}{1 + \lambda C(\sqrt{z})} G_C(0, x, z). \]  
As a straightforward consequence of this representation, the equation
\[ 1 + \lambda C(\sqrt{z}) = 0 \]  
determines the poles of the Green function, or in other words, the spectrum of eigenvalues of the Hamiltonian \( H_C + \lambda W(r) \).

Equation (37) can be written in the operator form:
\[ G(z) = G_C(z) - G_C(z) T(z) G_C(z), \]  
where the integral operator \( T(z) \) is defined by the kernel
\[ T(r, x, z) = \lambda \frac{\delta(r) \delta(x)}{1 + \lambda C(\sqrt{z})}. \]  
If now we formally introduce the Coulomb \( T \)-matrix by the representation of the Coulomb Green function
\[ G_C(z) = G_0(z) - G_0(z) T_C(z) G_0(z), \]  
where \( G_0(z) = (-\Delta - z)^{-1} \), then the equation (39) can further be rewritten in the standard form
\[ G(z) = G_0(z) - G_0(z) T(z) G_0(z). \]  
Here, \( T(z) \) is the \( T \)-matrix for Coulomb plus zero-range potentials given by the expression
\[ T(z) = T_C(z) + [I - T_C(z) G_0(z)] T(z) [I - G_0(z) T_C(z)]. \]  
This formula establishes the representation for the \( T \)-matrix in the case of the Coulomb plus zero-range interaction. It has the conventional form which follows from the standard two-potential formalism [16] if it is applied for the case of the superposition of the Coulomb and short-range potentials.

The formalism developed in the preceding part of the paper is used in the following sections for constructing a model for positron–electron interaction.
4. Electron–positron annihilation potential

The formula for the $2\gamma$ singlet $e^+e^-$ annihilation cross section derived from perturbative QED reads [19, 11]

$$\sigma_{\text{ann}} = \sigma_0 Z_{\text{eff}}, \quad (44)$$

where $\sigma_0 = \pi r_0^2 (c/v)$, $r_0$ is the classical electron radius, $c$ is the speed of light and $v$ is the incident velocity of the positron. The effective number of electrons $Z_{\text{eff}}$ participating in the annihilation is given by the integral

$$Z_{\text{eff}} = \int dr_1 dr_2 |\Psi^{0+}(r_1, r_2, r_p)|^2 \delta(r_1 - r_2). \quad (45)$$

Here, $\Psi^{0+}(r_1, r_2, r_p)$ (with $r_1$, $r_2$ and $r_p$ being the position vectors of the positron, the electron and the proton) is the solution of the positron–hydrogen scattering problem, when annihilation is not taken into account, and normalized in such a way that the incident wave has the form

$$\exp(ik_1 \cdot r_1)\Phi(r_2, r_p), \quad (46)$$

where $\Phi(r_2, r_p)$ is the hydrogen wavefunction.

In [10], to describe the absorption in the positron hydrogen scattering process, an imaginary optical potential of the form $i g W_{12}$, with $g < 0$, was introduced. The optical theorem, in the first-order Born approximation, gives the following expression for the absorption cross section:

$$\sigma_{\text{ann}}^B = \frac{-g}{k_1} \int dr_1 dr_2 W_{12}(r_1 - r_2) |\Psi^{0+}(r_1, r_2, r_p)|^2. \quad (47)$$

By comparing the QED expression (44) with equation (47) and taking into account that $\sigma_{\text{ann}} = \sigma_{\text{ann}}^B/4$ (the factor 1/4 comes from the fact that only singlet state is to be taken into account) it was proposed in [10] to determine the optical potential in such a way that it has the coupling constant of the form

$$g = -k_1 \sigma_0 \quad (48)$$

and the coordinate part of the form

$$W_{12}(r) = \delta(r), \quad (49)$$

where $r = r_1 - r_2$.

As we have discussed above, such a choice of the coordinate part of the potential leads to troubles in applications since the delta function as a potential can only be treated on the basis of the perturbation theory. Moreover, as it was studied in detail in [15], formula (47) is not valid for energies above the positronium formation threshold. In that paper, the use of the zero-range potential as a remedy for all of these problems has been proposed. Thus, the actual positron–electron annihilation potential in the framework of above considerations should be defined as

$$i g W_{12}(r) = i g W(r), \quad (50)$$

where $W(r)$ is the pseudo potential of equation (30). Consequently, the positron–electron Hamiltonian, which simultaneously describes the inter particle dynamics and annihilation, takes the form

$$H = H_C + i g W(r). \quad (51)$$
5. The positronium spectrum

In this section, we study the positronium spectrum as the discrete spectrum of the positron–electron Hamiltonian \( H_C + igW(\mathbf{r}) \) with annihilation potential \( (50) \). Here is the case when \( \epsilon = -1 \) in equation \( (9) \) and \( n < 0 \). The spectrum of \( H \) is formed by zeros of the denominator in \( (37) \) when \( \lambda = ig \). For analyzing the solutions of equation \( (38) \), we rewrite it in the form

\[
C(\sqrt{z}) = ig^{-1}. \tag{52}
\]

where

\[
C(\sqrt{z}) = \frac{i\sqrt{z}}{4\pi} + \frac{n}{4\pi} \left[ \log(-2i\sqrt{z}) + \psi \left( 1 + i \frac{n}{2\sqrt{z}} \right) + 2\gamma_0 - 1 \right]. \tag{53}
\]

Since the actual value of the coupling constant \( g \) is small, around \( 10^{-6} \) eV, we can seek the solution of equation \( (52) \) in the \( g \to 0 \) limit. In this limit, the right-hand side of \( (52) \) tends to infinity and so should the left-hand side. It may happen only due to the digamma function. Using the series expansion of the digamma function \[17\]

\[
\psi(x) = -\gamma_0 - \frac{1}{x} + \sum_{m=1}^{\infty} \left( \frac{1}{m} - \frac{1/m}{1+x/m} \right), \tag{54}
\]

we see that if the digamma function argument is equal to \(-m\), where \( m \) is a non-negative integer, then the left-hand side of equation \( (52) \) will obey the required property. Thus, we obtain the equation that determines the zero-order approximation to energy levels

\[
1 + i \frac{n}{2\sqrt{z}} = -m, \quad m = 0, 1, \ldots. \tag{55}
\]

Solving it, we recognize the pure Coulomb spectrum

\[
z_N = -\frac{n^2}{4N^2}, \quad N = 1, 2, \ldots \tag{56}
\]

in accordance with the obvious expectation when no absorption is present in the Hamiltonian if \( g = 0 \).

As the next stage, we will calculate the first-order correction to \( z_N \). First we represent the exact energy level in the form

\[
z_N' = -(\gamma_N + \delta_N)^2, \tag{57}
\]

where \( -\gamma_N^2 = z_N \) is the Coulomb energy and \( \delta_N \) is the correction of interest due to the presence of the annihilation potential. Obviously, we expect to have \( \delta_N = O(g) \). For calculating \( \delta_N \), let us use the inverse to equation \( (52) \)

\[
\frac{1}{C(\sqrt{z})} = -ig. \tag{58}
\]

According to the discussion above, the digamma function argument for values of \( z \) in the vicinity of \( z_N \) tends to a non-positive integer when \( g \to 0 \), i.e.

\[
1 + i \frac{n}{2\sqrt{z_N}} = 1 - N - \frac{n}{2\gamma_N^2} \delta_N + O(g^2) \quad N = 1, 2, \ldots. \tag{59}
\]

Due to equation \( (54) \) for the leading term of the digamma function when \( x \to -p \) with integer \( p \), we have

\[
\psi(x) \sim \frac{1}{x + p}, \quad p = 0, 1, \ldots. \tag{60}
\]
So, we can conclude that
\[ \frac{1}{\psi(1 + \frac{i n}{\sqrt{\kappa_1^2}})} = \frac{n}{2 \kappa_1^2} \delta_N + \mathcal{O}(g^2). \] 
(61)

where \( N = 1, 2, \ldots \). Now the left-hand side of equation (58) takes the form
\[ \frac{1}{C(\sqrt{z_N'})} = \frac{4\pi}{n \psi(1 + \frac{i n}{\sqrt{\kappa_1^2}})} + \mathcal{O}(g^2). \] 
(62)

Considering (61) we can rewrite this in the form
\[ \frac{2\pi}{\kappa_1^2} \delta_N + \mathcal{O}(g^2) = -ig, \] 
(63)

and for \( \delta_N \) we obtain
\[ \delta_N = -\frac{ig\kappa_1^2}{2\pi} + \mathcal{O}(g^2) = -\frac{ign^2}{8\pi N^2} + \mathcal{O}(g^2). \] 
(64)

Consequently, the energy levels are given by
\[ z_N' = -\kappa_1^2 - 2N\delta_N - \delta_N^2 = -\kappa_1^2 + ig \frac{(-n)^3}{8\pi N^3} + \mathcal{O}(g^2) \] 
(65)

with \( N = 1, 2, \ldots \). So we obtain the first-order correction to energy levels due to the annihilation potential
\[ ig \frac{(-n)^3}{8\pi N^3}, \quad N = 1, 2, \ldots. \] 
(66)

It is interesting to compare this value with the result of the standard perturbation theory. For the potential \( igW(r) \), the first-order energy level correction is given by the matrix element
\[ \langle \psi_{Nlm} | igW | \psi_{Nlm} \rangle = \int dr \psi_{Nlm}(r)igW(r)\psi_{Nlm}(r), \] 
(67)

where \( \psi_{Nlm}(r) \) is the Coulomb bound state wavefunction \[16\]:
\[ \psi_{Nlm}(r) = \sqrt{\frac{(-n)^3}{8 N^3}} \sqrt{\frac{(N - \ell - 1)!}{[(N + \ell)!]^3}} \exp \left[ \frac{nr}{2N} \right] \left( \frac{-nr}{N} \right)^\ell L_{2\ell+1}^\ell \left( -\frac{nr}{N} \right) Y_\ell^m(\theta, \phi). \] 
(68)

The integral on the right-hand side of (67) can easily be evaluated to give
\[ \langle \psi_{Nlm} | igW | \psi_{Nlm} \rangle = ig \psi_{Nlm}^2(0). \] 
(69)

Since \( \psi_{Nlm}^2(0) \) is non-trivial only for the s-wave, i.e. for \( l = 0 \), we have
\[ \psi_{N00}^2(0) = \frac{(-n)^3}{8\pi N^3}. \] 
(70)

This leads us to the final result for the perturbative correction:
\[ \langle \psi_{N00} | igW | \psi_{N00} \rangle = ig \frac{(-n)^3}{8\pi N^3}, \] 
(71)

which is in complete agreement with our previous result.
6. Electron–positron scattering

In this section, we consider the positron–electron scattering with annihilation. The latter is described by the annihilation potential \( igW(r) \). The corresponding wavefunction \( \psi(r, k) \) is the solution of the Schrödinger equation (12), with \( \lambda = ig \) and it possesses the asymptotic behavior as \( r \to \infty \):

\[
\psi(r, k) \sim \exp[ikr - i\eta \log(2kr)] f(\theta) \exp[ikr - i\eta \log(2kr)],
\]

where \( \theta \) is the scattering angle defined such that \( \cos \theta = r \cdot k/(rk) \) and \( f(\theta) \) is the scattering amplitude. As we have shown in section 2, this wavefunction satisfies the singular boundary condition at the origin

\[
\psi(0, k) = \frac{\alpha}{4\pi} [1/r + n \log r] + \beta + \mathcal{O}(r \log r)
\]

with \( \alpha/\beta = -ig \). It is also the solution of the integral equation (14) with \( \lambda = ig \), and consequently due to (15), (16) and (28) it can be written as

\[
\psi(r, k) = \psi_C(r, k) - ig \frac{\Gamma^2(1+i\eta) e^{-\pi \eta/2} W_{-i\eta;\frac{1}{2}}(-2ikr)}{1 + ig\eta C(k)} \frac{kr}{4\pi r}.
\]

By examining the asymptotic behavior of this wavefunction as \( r \to \infty \), we can determine the scattering amplitude \( f(\theta) \). The asymptotic expansion can be obtained from (74) by using the well-known asymptotic representations for the Coulomb wavefunction \( \psi_C(r, k) \) and the Whittaker function. The first term in (74) has the form of (72) with the Coulomb scattering amplitude [16]

\[
f_C(\theta) = -\frac{\eta}{2k \sin^2(\theta/2)} \exp[-i\eta \log(\sin^2(\theta/2))] + 2i\sigma_0. \tag{75}
\]

The Coulomb phase shift here is given by \( \sigma_0 = \arg \Gamma(1+i\eta) \). The asymptotics of the Whittaker function as \( r \to \infty \) reads [17]

\[
W_{-i\eta;\frac{1}{2}}(-2ikr) = e^{-\pi \eta/2} e^{i\pi \eta/2} \eta^{i\eta} + \mathcal{O}(1/r). \tag{76}
\]

Introducing these asymptotic representations into (74), we recover the asymptotic expansion (72) and as the result we obtain the exact representation for the scattering amplitude \( f(\theta) \)

\[
f(\theta) = f_C(\theta) + f'(\theta), \tag{77}
\]

where

\[
f'(\theta) = -\frac{ig}{4\pi} \frac{\Gamma^2(1 + i\eta) e^{-\pi \eta}}{1 + ig\eta C(k)}. \tag{78}
\]

The term \( f'(\theta) \) is the consequence of the annihilation potential and vanishes if \( g \to 0 \). Note that actually \( f' \) is angular independent, in accordance with the fact that the zero-range potential contributes only in the \( s \) partial wave.

As in the case of the positronium spectrum, this scattering amplitude can be compared with the result of the distorted wave Born approximation (DWBA). The first-order DWBA correction to \( f_C(\theta) \) is given by [16]

\[
f^B = -\frac{1}{4\pi} \int dr \psi_C(r, -k) gW(r) \psi_C(r, k), \tag{79}
\]

where \( \psi_C(r, k) \) is the scattering Coulomb wavefunction given by (11). The action of the pseudo potential \( W(r) \) on the Coulomb wavefunction can easily be evaluated:

\[
W(r) \psi_C(r, k) = \psi_C(0, k) \delta(r) = \Gamma(1+i\eta) e^{-\pi \eta/2} \delta(r). \tag{80}
\]

Thus, the integration in (79) results

\[
f^B = -\frac{ig}{4\pi} \Gamma^2(1 + i\eta) e^{-\pi \eta}. \tag{81}
\]

This, in fact, coincides with the leading term of our result of equation (78) as \( g \to 0 \).
7. Annihilation cross section

The total annihilation cross section accounts for the loss of flux due to annihilation. This loss is generated by the imaginary absorbing potential. In the case when \( H = -\Delta + V_1(r) + i g V_2(r) \), where \( V_1(r) \) and \( V_2(r) \) are short-range potentials, the scattering wavefunction has the asymptotic form

\[
\phi(r, k) \sim \exp[ikr] + A(\theta) \frac{\exp[ikr]}{r}.
\]

The optical theorem connects the imaginary part of the forward scattering amplitude to the total cross section \([16]\). If an absorption potential is present, then the standard form should be modified as \([15]\)

\[
\frac{4\pi}{k} \Im A(0) - \sigma = \frac{(-g)}{k} \int dr V_2(r) |\phi(r)|^2,
\]

where \( \sigma \) is the total cross section

\[
\sigma = 2\pi \int d\theta \sin^2 \theta |A(\theta)|^2.
\]

The right-hand side term of (82) is conventionally interpreted as the absorption cross section

\[
\sigma_a = \frac{(-g)}{k} \int dr V_2(r) |\phi(r)|^2.
\]

In the case of long-range potentials, when \( V_1(r) \) is the Coulomb potential, the left-hand side of the equation (82) is not well defined. The scattering amplitude in the forward direction is infinite and the integral (83) for the total cross section also diverges. The right-hand side should also be redefined if the pseudo potential is used for \( V_2 \). In order to obtain a generalization of the optical theorem (82) for Coulomb Hamiltonian with the zero-range potential, we consider the partial wave expansion in terms of Legendre polynomials \( P_\ell (\cos \theta) \):

\[
f(\theta) = \sum_{\ell=0}^\infty (2\ell + 1) f_\ell P_\ell (\cos \theta),
\]

where

\[
f_\ell = f^C_\ell + f'_\ell.
\]

Here the Coulomb partial amplitude reads

\[
f^C_\ell = \frac{\sin \sigma_\ell}{2ik},
\]

with \( \sigma_\ell = \arg \Gamma(\ell + 1 + i\eta) \). The additional amplitude \( f'_\ell \), which is due to the annihilation potential, vanishes for \( \ell \neq 0 \), and for \( \ell = 0 \) reads

\[
f'_0 = -\frac{ig}{4\pi} \frac{\Gamma^2(1 + i\eta) e^{-\pi\eta}}{1 + igC(k)}.
\]

The problems with the left-hand side of the optical theorem (82) in the Coulomb case come from the strong singularity of the Coulomb amplitude (75) in the forward scattering direction \( \theta = 0 \). This latter singularity is the consequence of the slow convergence of the series (85) \([20]\). In order to address this problem, let us truncate partial-wave expansions

\[
f_N(\theta) = \sum_{\ell=0}^N (2\ell + 1) f_\ell P_\ell (\cos \theta)
\]
\( \sigma_N = \sum_{\ell=0}^{N} 4\pi (2\ell + 1)|f_\ell|^2, \quad (90) \)

with \( N \) finite non-negative integer. Introducing the partial \( S \)-matrix elements

\( S_\ell = 1 + 2ikf_\ell, \quad (91) \)

we write the left-hand side of equation (82) as

\[ \frac{\pi}{k^2} \sum_{\ell=0}^{N} (2\ell + 1)(1 - |S_\ell|^2) = \frac{4\pi}{k} \Im m f_N(0) - \sigma_N. \quad (92) \]

If the absorption is absent, then the scattering is unitary, i.e. \( |S_\ell| = 1 \), and (92) yields

\[ \frac{4\pi}{k} \Im m f_N(0) - \sigma_N = 0. \quad (93) \]

As long as \( N \) is finite, this formula is valid for both short-range and long-range cases. The difference arises when one is attempting to calculate the limit \( N \to \infty \). Indeed, in the short-range case, the individual limits of each term on the left-hand side of (93) do exist and that leads to the standard optical theorem. However, in the long-range case, the individual limits do not exist, whereas the collective limit from (93) is immediate, and the optical theorem takes the form

\[ \lim_{N \to \infty} \left( \frac{4\pi}{k} \Im m f_N(0) - \sigma_N \right) = 0. \quad (94) \]

Let us consider now the case when besides the Coulomb potential an annihilation potential is also present. In this case, the \( S \)-matrix is not unitary, i.e. \( |S_0| \neq 1, |S_\ell| = 1 \) for \( \ell \geq 1 \). The latter reflects the fact that the zero-range potential is effective only in the \( s \)-wave.

More precisely, from equations (86)–(88) we have

\[ S_0 = e^{2i\sigma_0} + 2ikf_0', \quad (95) \]
\[ S_\ell = e^{2i\sigma_\ell}, \quad \ell \geq 1. \quad (96) \]

This leads for the left-hand side of (92)

\[ \frac{\pi}{k^2} \sum_{\ell=0}^{N} (2\ell + 1)(1 - |S_\ell|^2) = \frac{\pi}{k^2} (1 - |S_0|^2). \quad (97) \]

With this equation, we arrive at a variant of the optical theorem with finite \( N \):

\[ \frac{4\pi}{k} \Im m f_N(0) - \sigma_N = \frac{\pi}{k^2} (1 - |S_0|^2). \quad (98) \]

However, the right-hand side does not depend on \( N \). Hence, the \( N \to \infty \) limit of the left-hand side does exists and yields

\[ \lim_{N \to \infty} \left( \frac{4\pi}{k} \Im m f_N(0) - \sigma_N \right) = \frac{\pi}{k^2} (1 - |S_0|^2). \quad (99) \]

As in the case of standard optical theorem (82), the quantity on the right-hand side is a measure of the non-unitarity of the \( S \)-matrix and in our case it determines the annihilation cross section

\[ \sigma_{\text{ann}} = \frac{\pi}{k^2} (1 - |S_0|^2). \quad (100) \]

In order to finalize the generalization (99) of the optical theorem, we need to represent the right-hand side of (100) in terms of the wavefunction. This can be accomplished by using the exact representation (88) for the amplitude \( f_0' \) and the properties of the Coulomb
amplitudes. After some calculations, which are given in the appendix, we arrive at the desired representation

$$1 - |S_0|^2 = -\frac{g_k}{\pi} |\beta|^2,$$

which leads to the final form of the annihilation cross section

$$\sigma_{\text{ann}} = -\frac{g}{k} |\beta|^2$$

and to the final form of the optical theorem

$$\lim_{N \to \infty} \left( \frac{4\pi}{k} \Im m f_N(0) - \sigma_N \right) = -\frac{g}{k} |\beta|^2.$$ (103)

In previous sections, the parameter $\beta$ is represented through the wavefunction by the integral

$$\beta = \int dr W(r) \psi(r, k).$$ (104)

If the value of $\beta$ is calculated from this formula perturbatively, i.e. by using the leading term of $\psi$ when $g \to 0$, then we obtain

$$\psi(r, k) = \psi_C(r, k) + O(g)$$

and

$$\beta = \psi_C(0, k) + O(g).$$ (106)

Then for the annihilation cross section we have

$$\sigma_{\text{ann}} \sim -\frac{g}{k} \int dr \delta(r) |\psi_C(r, k)|^2$$

and for the optical theorem we obtain

$$\lim_{N \to \infty} \left( \frac{4\pi}{k} \Im m f_N(0) - \sigma_N \right) \sim -\frac{g}{k} \int dr \delta(r) |\psi_C(r, k)|^2.$$ (108)

8. Conclusion

In this paper, we have constructed the zero-range potential for the two-particle system with the Coulomb interaction. The Coulomb potential modifies the asymptotic behavior of the wavefunction at small distances. This asymptote has been studied with the help of the Lippmann–Schwinger integral equation. The pseudo potential has been constructed such that the wavefunction obeys the singular asymptotic boundary conditions. Although, the pseudo potential is constructed for the two-body case, its form is universal, and it can be used for several particle systems [21]. This work places the delta functional model of the annihilation potential [10] on a sound mathematical basis. The optical theorem, which formally cannot be formulated for charged particles, is reformulated in such a way it becomes applicable to the case of Coulomb plus imaginary absorbing potential of the zero range. This result facilitates the use of the annihilation potential for calculating annihilation in collision of positrons with atoms, including rearrangement processes with positronium formation [15].

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Appendix. Derivation of the representation for the annihilation cross section

Here we present the derivation of equation (101). Using the exact representations for the Coulomb phase shift and for $f'_0$, we obtain

$$1 - |S_0|^2 = -\frac{gk|\Gamma(1 + i\eta)|^2e^{-\pi\eta}}{\pi|1 + igC(k)|^2} - \frac{k^2|\Gamma(1 + i\eta)|^2e^{-\pi\eta}}{2\pi|1 + igC(k)|^2} \left\{ -2\Im mC(k) + \frac{k}{2\pi}|\Gamma(1 + i\eta)|^2e^{-\pi\eta} \right\}. \quad (A.1)$$

We show that the second term on the right-hand side is zero. Indeed, the first term in figure brackets can be transformed as

$$-2\Im mC(k) = -\frac{k}{2\pi} + \frac{n}{4} + \frac{n}{2\pi}\Im m\psi(1 + i\eta). \quad (A.2)$$

To proceed further, we use the formula [17]

$$\Im m\psi(1 + iy) = -\frac{1}{2y} + \frac{\pi}{2} \coth(\pi y) \quad (A.3)$$

to obtain

$$-\frac{k}{2\pi} + \frac{n}{4} - \frac{n}{2\pi}\Im m\psi(1 + i\eta) = -\frac{n}{2} \left( \frac{1}{e^{2\pi\eta} - 1} \right), \quad (A.4)$$

and therefore end up with

$$-2\Im mC(k) = -\frac{n}{2} \frac{1}{e^{2\pi\eta} - 1}. \quad (A.5)$$

Now, if we use in the term

$$\frac{k}{2\pi}|\Gamma(1 + i\eta)|^2e^{-\pi\eta} \quad (A.6)$$

the relation [17]

$$\Gamma(1 + iy)\Gamma(1 - iy) = \frac{\pi y}{\sinh(\pi y)}, \quad (A.7)$$

we obtain

$$\frac{k}{2\pi}|\Gamma(1 + i\eta)|^2e^{-\pi\eta} = \frac{n}{2} \frac{1}{e^{2\pi\eta} - 1}. \quad (A.8)$$

So, we have shown that the expression in figure brackets in (A.1) is equal to zero. Thus, we arrive at the equality

$$1 - |S_0|^2 = -\frac{gk|\Gamma(1 + i\eta)|^2e^{-\pi\eta}}{\pi|1 + igC(k)|^2} = -\frac{gk}{\pi}|\beta|^2, \quad (A.9)$$

which proves (101).

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