

## On the Regular Coulomb Functions. The Coulomb $T$ Matrix

Grigori Giorgadze<sup>a,b\*</sup> and Vagner Jikia<sup>b</sup>

<sup>a</sup>*I. Vekua Institute of Applied Mathematics of I. Javakishvili Tbilisi State University;*

<sup>b</sup>*I. Chavchanidze Institute of Cybernetics of Georgian Technical University*

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The two-particle regular Coulomb  $T$ -matrix of the continuous spectrum is described. It is rigorously shown that it exists in the sense of the generalized functions, and in the weak representation belongs to the set of Hilbert space functions. The above function satisfies the two-particle homogeneous integral equation of perturbation theory.

Due to its simple analytic structure and the correct properties, the obtained function is expected to be very useful for studying the standard singular integral equations of the scattering theory of several charged particles. Our calculations are carried out within the complex analysis using the modern non-standard methods.

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### 1. Motivation

It is well known the fact that the two-particle quantum-mechanical functions play an important role in the few-body problems. In particular, it is known that the kernel of the standard three-particle equations of the perturbation theory is determined by the Green's function of the free motion and the corresponding two-particle  $T$  matrices ([1], [2], pp. 51 - 54, see also [3], pp. 30 - 35). Let us note that the two-particle interaction  $T$  matrices in the three-particle equations appear outside the energy shell ([4], pp. 48 - 55). Accordingly, the properties and solvability of the above equations depend on the behavior of the input  $T$  matrices of this equations. At the same time, according to the three-particle formality, it is known that the off shell two-particle functions contain important information about the three-particle interactions ([5], pp. 267-269).

The investigations show that the fully off shell  $T$  matrices in the above three particle integral equations, in the case of the Coulomb field, have the singular behavior in the region of the half energy shell [6], [7]. Regularization of the  $T$  matrix with the above divergence using the latest standard methods, as well as the possibility its practical application in the problems with the few charged particles see, for instance in references ([8], [9] and therein).

Let us note the fact that the existence of the Coulomb functions in the momentum space was questionable for some time. Somewhat later, the opinion appeared

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\*Corresponding author. Email: gia.giorgadze@tsu.ge

that the above mentioned quantum-mechanical functions in the momentum space can be considered in the sense of the generalized functions. For instance, Van Haeringen and at al., studying the well-known asymptotic Coulomb functions of the continuous spectrum, announced that the functions under consideration exist in the momentum space in the sense of the generalized functions [7]. Investigating the integral representations of the mentioned functions, the similar conclusions were made by Anthony Chen ([10], pp. 41 - 51, see also pp. 63 - 67).

The connection of the Coulomb scattering operators with the singular generalized functions is also considered in the monograph [11]. In this work, it is shown that the functions Coulomb scattering on the unit sphere on the energy shell should be considered in the sense of generalized functions ([11], pp. 328 - 330, pp. 63 - 67).

Against the backdrop of the above scenario, it is interesting to note the Dušek renormalization method [12]. The author has shown that the regular fully off shell Coulomb  $T$  matrix  $\langle \vec{q} | T_C^+(k^2) | \vec{p} \rangle$  exists in the region of the point  $p = k$  and it is identical to the conventional half shell Coulomb  $T$  matrix with the following well-known integral representation (see also [13]):

$$\langle \vec{q} | T_C^+ | \vec{k} \rangle = \int_0^{+\infty} \exp(-i\vec{q}\vec{r}) V_C(r) \psi_C^+(\vec{r}, \vec{k}) d\vec{r}. \quad (1)$$

The function  $V_C(r)$  in the above representation is the Coulomb potential of the central interaction, and  $\psi_C^+$  is the Coulomb scattering function with the outgoing boundary condition ([14], pp. 569 - 570).

Note the fact that due to the weak convergence of the potential  $V_C$  the infrared divergence appears in the expression (1). Accordingly, the  $T$  matrix mentioned above doesn't exist in the functional sense ([10], pp. 21 - 29).

At the same time, there is the point of view that the diagonal element of the  $T$  matrix of the Coulomb scattering is equal to zero. Gerald Nutt was one of the first to propose the opinion mentioned above [15]. The correct mathematical confirmation of the Nutt's idea was done by West and Shustri and Rajagopal [16], [17]. In connection with this issue, it is also interesting to note the studies and opinions that are given in the following article [7].

A rigorous mathematical formulation of the above opinion using non-standard methods will be proposed in details in the near future. Some of the obtained main results will be briefly described below in this paper.

As we have mentioned, the formalism represented in this article was motivated by recent and numerous calculations within the complex analysis. For instance, see the following references [18], [19], [20], [21], [22].

From the obtained results, we would like to note the calculations that concern the Euler-type singular integrals [18], as they can be used as the basis for the correct mathematical theory of the mentioned integrals.

For instance, in the above papers it is shown that the singular integral

$$B(i\gamma - m, -i\gamma - n) = \int_0^1 t^{i\gamma - m - 1} (1 - t)^{-i\gamma - n - 1} dt, \quad (2)$$

where  $m$  and  $n$  are integer numbers ( $m \geq 0$  and  $n \geq 0$ ), exists in the sense of the

generalized functions and can be expressed by the Dirac delta function [18].

In the case when  $m = n = 0$  the integral (2) takes the following form [19]:

$$B(i\gamma, -i\gamma) = \int_0^1 t^{i\gamma-1} (1-t)^{-i\gamma-1} dt = 2\pi\delta(\gamma). \quad (3)$$

The recent studies show that the formula (3) together with the other calculations [20], [21] plays an important role in the quantum mechanics of two charged particles of the continuous spectrum. Details will be published shortly.

Besides of the scenario described above, there are numerous studies which confirm that the Coulomb functions of the continuous spectrum at the point  $q = k$  and its vicinity are characterized by incorrect behavior [7], [23], [24], [25], [26], [27], see also ([10], pp. 22 - 36). At the same time, as we have mentioned, the recent calculations within the non-standard approach show that there are the regular Coulomb functions of the Hilbert space ( $L_2$ ) of the continuous spectrum which vanish at the point  $q = k$  and its vicinity. Note that the regular functions mentioned above outside the neighborhood of the point  $q = k$  are well-defined analytic functions.

We hope that the calculations and opinions proposed in this article will be interesting against the backdrop of the ambiguous representations that currently exist in the scattering theory of two charged particles [7], [11], [16], [17], see also ([28], pp. 513 - 516 and therein).

## 2. The regular Coulomb $T$ matrix

Since the integral (1) doesn't exist in a functional form, we used the following well-known limit to study the Coulomb  $T$  matrix [24]:

$$\langle \vec{q} | T_C^+ | \vec{k} \rangle = \int_0^{+\infty} \exp(-i\vec{q}\vec{r} - \alpha r) V_C(r) \psi_C^+(\vec{r}, \vec{k}) d\vec{r}, \quad \alpha \rightarrow 0 \quad (4)$$

and by the precise calculations, the following result is obtained.

**Theorem 2.1:** *The Coulomb  $T$  matrix, defined by the integral formula (4), can be formally expressed as follows:*

$$\langle \vec{q} | T_C^+ | \vec{k} \rangle = H(\xi^2 - \lambda^2) T_C^+(\vec{q}, \vec{k}) + \tilde{H}(\xi^2 - \lambda^2) \tilde{X}_C^+(\vec{q}, \vec{k}). \quad (5)$$

where  $T_C^+$  is the analytical function, and  $\tilde{X}_C^+$  is expressed by the functionals.

**Remark 1:** The function  $H(x)$  in the expression (5) is the Heaviside Unit function, which is determined in the following manner ([29], pp. 77 - 81):

$$H(\xi^2 - \lambda^2) = \begin{cases} 1 & \xi^2 - \lambda^2 > 0 \\ 0 & \xi^2 - \lambda^2 \leq 0 \end{cases} = \begin{cases} 1 & |\xi| > \lambda, \\ 0 & |\xi| \leq \lambda, \end{cases} \quad \lambda > 0, \\ \xi = q - k, \quad 0 < \lambda \ll 1.$$

The function  $\tilde{H}(x)$  in the equality (5) is defined as follows:

$$\tilde{H}(\xi^2 - \lambda^2) = 1 - H(\xi^2 - \lambda^2).$$

Let us note, that the parameter  $\lambda$  separates the small region  $[k - \lambda, k + \lambda]$  of the point  $q = k$  from the rest of the impulse space.

Note also that it isn't necessary to separate the area of the point  $q = k$  from the rest of the impulse space in the symmetric boundaries.  $\square$

Expanding into the partial waves, in the area of the point the  $q = k$ , the matrix  $T$  under consideration can be expressed in terms of the following series:

$$\begin{aligned} \tilde{X}_C^+(\vec{q}, \vec{k}) &= \sum_l (2l + 1) X_C^+(q, k) P_l(\cos \theta), \quad \cos \theta = \hat{q} \cdot \hat{k}, \\ q &\in [k - \lambda, k + \lambda]. \end{aligned} \quad (6)$$

To estimate the behavior of the second summand in the expression (5), let us rewrite the functional (6) in the weak representation.

Let us take into account that in the coefficients of the series (6) the arguments  $q$  and  $k$  enter in the form of the following ratio:

$$X_C^+(q, k) \equiv X_C^+(q/k), \quad q \in [k - \lambda, k + \lambda]. \quad (7)$$

Using the substitution:  $q = k + \tau$  in the expression (7) and taking into account the relation  $\gamma = -1/k$ , the above identity can be rewritten in the following explicit form with respect to the arguments:

$$\begin{aligned} X_C^+\left(\frac{\tau\gamma - 1}{\gamma}, -\frac{1}{\gamma}\right) &\equiv X_C^+(1 - \tau\gamma) \equiv X_C^+(\tau, -\gamma), \\ |\tau| &\leq \lambda, \quad 0 < \lambda \ll 1. \end{aligned} \quad (8)$$

According to the latest calculations, we have:

$$X_C^+(\tau, -\gamma) = 2^{-1} \pi \gamma^2 \delta(\gamma) + \mathcal{O}(-\tau\gamma), \quad |\tau| \leq \lambda, \quad (9)$$

where the small quantity  $\mathcal{O}$  vanishes at the point  $\tau = 0$ .

Let's rewrite the functional (9) in the integral form.

In the above weak representation, we obtain the following correct definition:

$$X_C^+(\tau, -\gamma) := X_R^+(\tau, \varphi), \quad |\tau| \leq \lambda, \quad (10)$$

where the quantity  $X_R^+(\tau, \varphi)$  is defined as follows:

$$X_R^+(\tau, \varphi) = 2^{-1}\pi \int_{-a}^a \gamma^2 \delta(\gamma) \varphi(\gamma) d\gamma \tag{11}$$

$$+ \int_{-a}^a \mathcal{O}(-\tau\gamma) \varphi(\gamma) d\gamma, \quad 0 < a < \infty,$$

$$|\tau| \leq \lambda, \quad 0 \leq |\tau\gamma| \ll 1, \quad 0 < \lambda \ll 1.$$

In the formula (11) it is assumed that  $0 < k$ . Accordingly, the spectrum of the  $\gamma$  parameter is changeable in the following area;  $-a < |\gamma| < a$ .

The calculations show that there exists the set of the well defined functions for which the following equalities hold in the area of the point  $q = k$ :

$$X_R^+(\tau, \varphi) \equiv X_R^+(\tau), \quad X_R^+(\tau) = \tilde{\mathcal{O}}(\tau), \quad |\tau| \leq \lambda. \tag{12}$$

The infinitesimal quantity  $\tilde{\mathcal{O}}$ , as in the case of the expression (9), satisfies the following condition:  $\tilde{\mathcal{O}}(0) = 0$ .

According to the formulas (7), (8) and (10) we obtain the following definition of the coefficients of the expansion (6) in the weak sense:

$$X_C^+(q/k) \equiv X_C^+(1 - \tau\gamma) := X_R^+(\tau), \quad |\tau| \leq \lambda. \tag{13}$$

Thus, according to the expression (9), the expansion coefficients of the function (5) in the region of the point  $q = k$  can be expressed in terms of the generalized function, which in the weak representation (10) determines ([30], pp. 235 - 251) the correct radial part (13) of the considered expansion (6) in the domain under consideration.

For convenience, instead of the pair  $(\tau, \gamma)$ , that we have used in the formulas (8) - (13), the arguments  $q$  and  $k$  will be applied again in the expressions below.

Using the definition (13) in the decomposition (6), we obtain the following singularity with respect to the angular variables:

$$X_C^+(\vec{q}, \vec{k}) = X_C^+(q/k) \delta(\hat{q} - \hat{k}), \quad q \rightarrow k. \tag{14}$$

The formula (14) shows that the series (6) with the correct radial part (13) is the functional with respect to the angular variables.

To obtain the regular  $T$  matrix, let represent the functional (14) in the weak sense with respect to angular variables by the following formal way:

$$X_R^+(\vec{q}, \vec{k}) \stackrel{weak}{=} X_C^+(\vec{q}, \vec{k}), \quad q \rightarrow k. \tag{15}$$

Using the formal expression (15), the results of the regularization procedure (4) can be formulated in the following form.

**Theorem 2.2:** *The two-particle Coulomb  $T$  matrix of the continuous spectrum*

(5) can be formally represented in the following correct form:

$$\langle \vec{q} | T_R^+ | \vec{k} \rangle = H(\xi^2 - \lambda^2) T_C^+(\vec{q}, \vec{k}) + \tilde{H}(\xi^2 - \lambda^2) X_R^+(\vec{q}, \vec{k}), \quad (16)$$

where  $T_C^+$  is the well-defined analytical function, and  $X_R^+$  is the infinitesimal quantity, determined in the weak representation.

Due to the expressions (16) and (15) one can determine the regular Coulomb  $T$  matrix in the region of the energy shell ( $q = k$ ) as follows:

$$\langle \vec{q} | T_R^+ | \vec{k} \rangle \stackrel{weak}{=} X_C^+(\vec{q}, \vec{k}), \quad q \rightarrow k. \quad (17)$$

Thus, we have defined the regular  $T$  matrix by the weak equalities (17) and (13). That is, we expressed the functional (6) in the weak sense to determine the  $T$  matrix under consideration in the region of the energy shell ( $q = k$ ).

Using the formal expression (17), let us define the radial part of the function (16) in the region under consideration.

To this end, let us rewrite the expression (17) in the explicit form:

$$\int_{\Omega} \langle \vec{q} | T_R^+ | \vec{k} \rangle f(\hat{q}) d\hat{q} = \int_{\Omega} X_C^+(\vec{q}, \vec{k}) f(\hat{q}) d\hat{q}, \quad q \rightarrow k. \quad (18)$$

The basis function  $f(\hat{q}) = C \cdot f(\hat{q})$  in the equality (18) is well defined (belongs to the set of the Schwartz functions) and satisfies the following condition:

$$C \int_{\Omega} \delta(\hat{p} - \hat{k}) f(\hat{p}) d\hat{p} = 1. \quad (19)$$

Let's expand the weak expression (18) in partial waves.

Substituting the expansion (14) into the weak equality (18), one can write:

$$\int_{\Omega} \langle \vec{q} | T_R^+ | \vec{k} \rangle f(\hat{q}) d\hat{q} = X_C^+(q/k) \int_{\Omega} \delta(\hat{q} - \hat{k}) f(\hat{q}) d\hat{q}, \quad q \rightarrow k. \quad (20)$$

Expanding the right side of the expression (20) in terms of the partial waves and taking into account the condition (19), we obtain:

$$\langle q | T_R^+ | k \rangle := X_C^+(q/k), \quad q \rightarrow k, \quad (21)$$

where the function  $X_C^+$  is defined by the relations (13).

Thus, by decomposing the expression (18) in terms of the partial waves we got the desired radial function (21).

According to the equality (21), the regular  $T$  matrix (16), in the region of the point  $q = k$  represents the infinitesimal quantity (12), depending on the scalar value. In addition, the considered  $T$  matrix in the above region is expressed by the expansion coefficients of the series (6) in the weak representation (13).

Moreover, we want to note the fact that the Coulomb  $T$  matrix (16) in the region of the energy shell  $q = k$  does not depend on the quantum number  $l$ . Furthermore, recall that the small quantity mentioned above vanishes at the point  $q = k$ .

The regular  $T$  matrix (16) outside the energy shell ( $q = k$ ) coincides with the function (5) and represents the exact analytical function  $T_C^+(\vec{q}, \vec{k})$ .

The above function is defined by the following series:

$$T_C^+(\vec{q}, \vec{k}) = \sum_l (2l+1) T_{Cl}^+(q, k) P_l(\cos \theta), \quad \cos \theta = \hat{q} \cdot \hat{k}, \quad (22)$$

$$q \in [0, k - \lambda \cup] k + \lambda, \infty].$$

The expansion coefficients in the series (22) have the following exact form:

$$T_{Cl}^+(q, k) = C_l(\gamma) V_{Cl}(q, k), \quad q \in [0, k - \lambda \cup] k + \lambda, \infty], \quad (23)$$

where  $C_l$  is the complex number and the function  $V_{Cl}(q, k)$  which denotes the radial part of the Coulomb potential of two-particle interaction in the impulse space in the center of mass system of the interacting particles. The function  $V_{Cl}(q, k)$  in the Hartree system of units can be expressed as follows:

$$V_{Cl}(q, k) = \frac{1}{2qk} Q_l \left( \frac{q^2 + k^2}{2qk} \right).$$

Thus, according to the scenario described above, the radial part of the considered  $T$  matrix (16) is formally defined as follows:

$$\langle q | T_{Rl}^+ | k \rangle := H(\xi^2 - \lambda^2) T_{Cl}^+(q, k) + \tilde{H}(\xi^2 - \lambda^2) X_C^+(q/k), \quad (24)$$

where the off shell function  $T_{Cl}^+(q, k)$  is expressed by the equality (23), and the expression  $X_C^+(q/k)$  is determined by the formulas (13) and represents the infinitesimal quantity, which vanishes on the energy shell ( $q = k$ ).

It can be shown that the Coulomb scattering matrices (24) and, accordingly, (16) satisfy the following condition:

$$L_2(R) = \left\{ T_R^+ : R \rightarrow C \mid \int_0^\infty |\langle \vec{q} | T_R^+ | \vec{k} \rangle|^2 d\vec{q} < \infty \right\},$$

and, respectively, belong to the set of vectors of the Hilbert space  $L_2$ .

According to the scenario described above, the full set of the quantum mechanical states (16) vanishes at the point ( $q = k$ ) and its vicinity.

Note that the considered  $T$  matrix has the following important property.

**Theorem 2.3:** The  $T$  matrix (16) satisfies the following two-particle standard integral equation of the perturbation theory

$$\langle \vec{q} | T_R^+ | \vec{k} \rangle = \int_0^\infty V_C(\vec{q} - \vec{p}) \frac{g}{k^2 - p^2 + i\varepsilon} \langle \vec{p} | T_R^+ | \vec{k} \rangle d\vec{p} \quad (25)$$

with the weak singular Coulomb potential  $V_C$ .

One can show that the equation (25) with the singular Coulomb kernel vanishes in the energy shell region and, respectively, is correct.

Thus, the scenario described above represents the rigorous mathematical confirmation of the fact that the Coulomb functions of the continuous spectrum exist in the region of the point  $q = k$  in the sense of generalized functions [7].

### 3. Conclusions

Thus, according to the recent calculations, the well-known Coulomb representation (4) defines the regular function of the continuous spectrum of the Hilbert space (16), which in the energy shell region ( $q \rightarrow k$ ) is determined in the weak sense (17). The function under consideration satisfies the two-particle homogeneous standard integral equation of the perturbation theory (25).

Note that the approach described above also provides for the regularization of the Coulomb potential and the Fourier image of the Coulomb wave function, therefore it is possible to formulate the systematic consistent mathematical theory of two charged particles of the continuous spectrum.

The scenario described above also gives the perspective to construct the unified formalism for atomic and nuclear two-particle collisions at the low energy kinematics. Furthermore, it is interesting to generalize the above approach for investigations of the relativistic (Dirac) electron.

Let us notice that the obtained results are important not only from the theoretical point of view but also for practical applications. In particular, the function (16) is interesting not only for its correct properties, but also due to its simple structure. Accordingly, the considered function allows us to eliminate inaccuracies in the problems of the scattering of several charged particles, and then it can be conveniently used while performing specific calculations in these problems.

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