Coulomb screening in the momentum-space description of proton-deuteron elastic scattering: Examination of the need for renormalization

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Proton-deuteron elastic scattering is considered in the framework of momentum-space Faddeev equations with the screening method for the Coulomb interaction. It is shown how the interplay of the proton-proton Coulomb potential and the deuteron pole in the neutron-proton transition operator leads to coinciding singularities in the Faddeev equation. The coincidence of those singularities was not taken into account in a previous work [Witała *et al.*, Eur. Phys. J. A **41**, 369 (2009)], leading to a conjecture that no renormalization is needed. However, the coinciding singularities closely resemble those of the point deuteron-proton system, naturally suggesting that the renormalization of the scattering amplitude is needed in the unscreened Coulomb limit and can be performed conveniently in terms of the point deuteron-proton system.

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I. INTRODUCTION

The proton-deuteron scattering in the momentum-space framework is often described employing the screening of the Coulomb potential, thereby rendering it of short range and treatable by the standard scattering theory. However, there is no consensus in the literature regarding the behavior and renormalization of amplitudes in the unscreened limit. For example, while the most studies [1–4] require the renormalization of scattering amplitudes, the work by Witała *et al.* [5] claims the existence of the unscreened limit for the proton-deuteron elastic scattering amplitude without renormalization. The present work tries to explain those differences.

II. COULOMB SCREENING AND RENORMALIZATION

The long-range nature of the Coulomb interaction prevents the direct application of the standard scattering theory. In the momentum space the Coulomb potential

$$\langle \mathbf{p}_f|w|\mathbf{p}_i\rangle \equiv w(\mathbf{p}_f - \mathbf{p}_i) = \frac{\alpha}{(\mathbf{p}_f - \mathbf{p}_i)^2} \tag{1}$$

is singular for the vanishing momentum transfer. In the Lippmann-Schwinger equation for the two-body transition operator

$$\begin{aligned}\langle \mathbf{p}_f|t_c\big(p_o^2/2\mu + i0\big)|\mathbf{p}_i\rangle \\ = \frac{\alpha}{(\mathbf{p}_f - \mathbf{p}_i)^2} + \int d^3p \, \frac{\alpha}{(\mathbf{p}_f - \mathbf{p})^2} \\ \times \frac{2\mu}{p_o^2 - p^2 + i0}\langle \mathbf{p}|t_c(p_o^2/2\mu + i0)|\mathbf{p}_i\rangle\end{aligned} \tag{2}$$

this potential singularity coincides with the singularity of the free resolvent, if the half-shell condition $p_f = p_o$ is fulfilled. Although integrable separately, the coinciding singularities become nonintegrable. As a consequence, the equation is ill defined and the standard scattering amplitude does not exist. In the above equations $\alpha = \alpha_{\text{e.m.}}/2\pi^2$ with $\alpha_{\text{e.m.}} \approx 1/137$ being the fine structure constant, μ is the reduced mass and $\mathbf{p}_j$ denote the relative two-particle momenta.

The problem can be solved by introducing the screening of the Coulomb potential at large distances $r > R$ in the coordinate space, rendering the momentum-space potential nonsingular, then solving the Lippmann-Schwinger equation and taking the unscreened Coulomb, i.e., $R \to \infty$ limit [6]. It was shown that in the $R \to \infty$ limit the half-shell and on-shell matrix elements of the transition operator acquire a diverging phase factor [6]. After the isolation and removal of that factor, the so-called renormalization, the resulting amplitudes are well behaved (at least as distributions), and can be used to calculate scattering observables in a standard way. The procedure can be extended when the additional short-range forces are present: the troublesome Coulomb contributions are isolated such that the diverging phase factor to be removed via the renormalization is known from the pure Coulomb problem [7].

The idea of screening and renormalization has been applied also for the three-body problem; see Refs. [1–4] for a detailed description. In short, full three-body transition operators are decomposed such that the problematic Coulomb contributions are isolated. In the proton-deuteron elastic scattering this is achieved by introducing auxiliary two-body operators driven by the screened Coulomb force between the proton and the center of mass of the deuteron. Being solutions of the two-body Coulomb problem, these operators display the corresponding behavior in the $R \to \infty$ limit where the diverging phase factor is known and can be removed via the renormalization. It must be emphasized that these auxiliary operators do not imply approximating the proton-proton Coulomb force

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by the proton-deuteron one. In the solved three-body equations the Coulomb force between the protons is included. Witała *et al.* [5] have chosen a slightly different strategy. They started with the symmetrized three-nucleon Faddeev equation in the isospin formalism, where the two-body proton-proton transition operators contained also Coulomb contributions. Without introducing auxiliary operators, they investigated the behavior of all terms in the Faddeev equation and concluded the absence of strong singularities for the elastic amplitude. This led to the conclusion that the proton-deuteron elastic scattering amplitude should exist without renormalization.

In contrary to Ref. [5], it will be shown here that also without the introduction of the auxiliary operators the proton-deuteron elastic scattering equation in the unscreened Coulomb limit has coinciding singularities of the same type as in the two-body problem (2). There is no intention to provide a complete rederivation of the proton-deuteron formalism, which is already given in Refs. [1–4]; the Faddeev equation of Ref. [5] is not the optimal starting point for this purpose.

In the following, the dependence on the Coulomb screening radius R is suppressed in the notation, having the unscreened limit $R \to \infty$ in mind. The Faddeev equation in the Alt-Grassberger-Sandhas (AGS) version [8] for the symmetrized proton-deuteron transition operator

$$U = PG_0^{-1} + PtG_0U \tag{3}$$

after one iteration becomes

$$U = PG_0^{-1} + PtP + PtG_0PtG_0U. \tag{4}$$

Here G_0 is the free resolvent, t is the two-nucleon transition operator, and P is the sum of two cyclic permutation operators [4]. Isospin formalism is used, meaning that for given isospin states the t operator is a linear combination of proton-neutron and proton-proton operators, the latter including also the Coulomb contribution. For calculation of elastic scattering observables one needs the matrix elements of U between the proton-deuteron states $|\phi_d \mathbf{q}_j\rangle$ where ϕ_d denotes the deuteron wave function with the binding energy ϵ_d, and $\mathbf{q}_j$ denotes the relative spectator-pair momentum. The dependence on the discrete quantum numbers is suppressed in the notation. With explicit intermediate integrations the third term in Eq. (4) then reads

$$\int \langle \phi_d \mathbf{q}_f | PtP | \mathbf{pq}\rangle d^3p\, d^3q \langle \mathbf{pq}|G_0tG_0|\mathbf{p}'\mathbf{q}'\rangle d^3p'\, d^3q' \times \langle \mathbf{p}'\mathbf{q}'|U|\phi_d\mathbf{q}_i\rangle. \tag{5}$$

The structure of this integrand will be investigated in the proton-deuteron on-shell limit for q, that is, $q \to q_o$, where q_o is the relative proton-deuteron on-shell momentum, corresponding to the system energy in the c.m. frame $E = q_o^2/2\mu_{pd} - \epsilon_d$. Near this q value the matrix elements of the free resolvent G_0 are finite, but the two-nucleon transition operator has a pole corresponding to the deuteron bound state, i.e.,

$$\langle \mathbf{pq}|G_0tG_0|\mathbf{p}'\mathbf{q}'\rangle \xrightarrow[q\to q_o]{} \langle \mathbf{p}|\phi_d\rangle \frac{2\mu_{pd}\,\delta(\mathbf{q}-\mathbf{q}')}{q_o^2 - q^2 + i0}\langle\phi_d|\mathbf{p}'\rangle. \tag{6}$$

Thus, in the vicinity of $q \to q_o$ the contribution of the deuteron pole to (5) is

$$\int \langle \phi_d\mathbf{q}_f|PtP|\phi_d\mathbf{q}\rangle d^3q\, \frac{2\mu_{pd}}{q_o^2 - q^2 + i0}\langle\phi_d\mathbf{q}|U|\phi_d\mathbf{q}_i\rangle. \tag{7}$$

The matrix element $\langle \phi_d\mathbf{q}_f|PtP|\phi_d\mathbf{q}\rangle$, appearing also as the second term in Eq. (4), in the isospin formalism has contributions from proton-proton and neutron-proton t operators, which are fully off shell under the $q \to q_o$ condition. The nonsingular contributions are omitted in the following. In the unscreened Coulomb limit $R \to \infty$ the singular part of this matrix element arises from the off-shell proton-proton transition operator t_c^R contained in t whose singularity is the same as in the proton-proton Coulomb potential [9]. Thus, when investigating the structure of singularities one can replace t by $\frac{2}{3}\,w$, where the $\frac{2}{3}$ factor arises from the isospin weighting [4]. The result has the form

$$\tfrac{2}{3}\langle\phi_d\mathbf{q}_f|PwP|\phi_d\mathbf{q}\rangle = w(\mathbf{q}_f - \mathbf{q})\,F_1(\mathbf{q}_f - \mathbf{q}) + F_2(\mathbf{q}_f, \mathbf{q}), \tag{8}$$

where the regular form-factor-type functions F_k involve spin-coupling coefficients and integrals over the deuteron wave function (F_2 involves also the Coulomb potential, but its singularity is integrated out). Detailed expressions for F_k are irrelevant, except for the particular feature $F_1(0) = 1$. This means that in the limit of the vanishing momentum transfer $\mathbf{q}_f \to \mathbf{q}$, the singular part of (8) is exactly the same as in the proton scattering off a point deuteron. Combining together expressions (6) and (8) in the unscreened Coulomb limit and leaving out regular terms one arrives at

$$\int d^3q\, \frac{F_1(\mathbf{q}_f - \mathbf{q})}{(\mathbf{q}_f - \mathbf{q})^2}\, \frac{2\mu_{pd}}{q_o^2 - q^2 + i0}\,\langle\phi_d\mathbf{q}|U|\phi_d\mathbf{q}_i\rangle. \tag{9}$$

Obviously, in the proton-deuteron on-shell limit $q_f = q_o$ the two singularities in (9) coincide, the integral does not converge. Furthermore, the structure of singularities is the same as in the two-body pure Coulomb problem (2). One may also note that second term of (4), PtP, at $q_f = q_o = q_i$ and $\mathbf{q}_f \to \mathbf{q}_i$ would include an infinite contribution (8) to the forward scattering amplitude. It does not carry a diverging phase factor, resembling the proton-deuteron Coulomb potential rather than the Rutherford amplitude. Thus, there is a close similarity with the two-body (proton + point deuteron) scattering problem involving short-range and Coulomb forces, and one may expect similar mathematical properties when applying the method of Coulomb screening. In particular, the proton-deuteron elastic scattering amplitudes would acquire diverging phase factors in the $R \to \infty$ limit and would necessitate the renormalization. Based on the above equations, one could expect the proton scattering off a point deuteron to be the reference problem that determines renormalization factors and direct Coulomb amplitude, as the effective charge, momenta, and reduced mass correspond exactly to those of the (proton + point deuteron) system. Noteworthy, this conjecture is achieved without introducing auxiliary proton-deuteron operators. Thus, the renormalization in terms of the (proton + point deuteron) system is not introduced artificially but emerges naturally from the analysis of singularities.

As the above derivation was not relying on the properties of the initial state $|\phi_d \mathbf{q}_i\rangle$, the singularity structure made explicit in (9) obviously persists for any initial momentum $\mathbf{q}_i$ and the pair state with relative momentum $\mathbf{p}_i$. In analogy with the two-body problem this again implies that not only the on-shell but also the half-shell matrix elements $\langle \phi_d \mathbf{q}_f | U | \mathbf{p}_i \mathbf{q}_i \rangle$ at $q_f = q_o \neq q_i$ need an appropriate renormalization. The initial-final state symmetry of the transition operator U suggests the necessity of the renormalization also at $q_i = q_o \neq q_f$. The singularity structure at $q_i = q_o$ can be easily shown to be of the type (9). For this one could start with an alternative form of the AGS equation

$$U = PG_0^{-1} + UG_0 tP \tag{10}$$

and repeat similar steps as given in (4)–(8) for the half-shell matrix element $\langle \mathbf{p}_f \mathbf{q}_f | U | \phi_d \mathbf{q}_i \rangle$, arriving at

$$\int d^3q \, \langle \mathbf{p}_f \mathbf{q}_f | U | \phi_d \mathbf{q} \rangle \, \frac{2\mu_{pd}}{q_o^2 - q^2 + i0} \, \frac{F_1(\mathbf{q} - \mathbf{q}_i)}{(\mathbf{q} - \mathbf{q}_i)^2} \tag{11}$$

instead of (9), with coinciding singularities at $q_i = q_o$.

The fact that half-shell matrix elements $\langle \mathbf{p}_f \mathbf{q}_f | U | \phi_d \mathbf{q}_i \rangle$ at $q_i = q_o$ need an appropriate renormalization implies a corresponding property also for operator products acting on $U|\phi_d \mathbf{q}_i\rangle$. In particular, the Faddeev operator of Ref. [5]

$$tG_0U \equiv T = tP + tG_0PT, \tag{12}$$

when acting on the initial proton-deuteron state with $q_i = q_o$, i.e., $T|\phi_d \mathbf{q}_i\rangle = tG_0U|\phi_d \mathbf{q}_i\rangle$, at least needs a renormalization associated with the initial state. The elastic amplitude [5] is

$$\begin{aligned} &\langle \phi_d \mathbf{q}_f | \big(PG_0^{-1} + PT\big) | \phi_d \mathbf{q}_i \rangle \\ &\quad = \langle \phi_d \mathbf{q}_f | PG_0^{-1} | \phi_d \mathbf{q}_i \rangle + \langle \phi_d \mathbf{q}_f | PtP | \phi_d \mathbf{q}_i \rangle \\ &\qquad + \langle \phi_d \mathbf{q}_f | PtPG_0T | \phi_d \mathbf{q}_i \rangle, \end{aligned} \tag{13}$$

where one can easily identify the three terms in (4), a consequence of the equivalence between the AGS equation (3) for U and the Faddeev equation (12) for T. In particular, since in the two-nucleon ${}^3S_1 - {}^3D_1$ wave the operator T carries the deuteron bound-state pole as t does, the singularity structure of the third term in (13) is exactly the same as in (9), i.e., the two singularities from the proton-proton Coulomb potential and the deuteron pole do coincide, such that the renormalization in the unscreened limit of (13) is needed also for the final state. Alternatively, for convenience one may introduce a reduced form of T with the deuteron pole separated from T as Refs. [5,10] do, but then the deuteron pole has to be included explicitly in the last term for the elastic amplitude (13) leading to exactly the same result. On the other hand, looking back to the left-hand sides of (12) and (13) it is quite obvious that off-shell T exhibits singular behavior itself, stemming from the off-shell t_c^R.

III. DISCUSSION

The above consideration is not a rigorous proof of the screening and renormalization procedure for the proton-deuteron scattering, see Refs. [2,4] instead. However, it demonstrates one more time that in the proton-deuteron scattering problem one encounters typical difficulties related to the Coulomb treatment, manifesting themselves by coinciding singularities in the momentum-space framework. This feature arises not from the proton-proton transition operator directly, but via the interplay between the proton-proton Coulomb interaction and the deuteron bound-state pole. In fact, one may consider the energy regime below the deuteron breakup threshold where the two-nucleon transition operators are always off shell at negative two-nucleon energies, and do not need renormalization. However, even in this case the coinciding singularities (9) persist and, consequently, the proton-deuteron elastic scattering amplitudes need renormalization.

It is very important to note that the work by Witała *et al.* [5] disregarded the appearance of coinciding singularities by interplay of the proton-proton Coulomb potential and the deuteron pole. In Sec. 4 of Ref. [5] Witała *et al.* considered only the singularities and renormalization features of the half-shell and on-shell proton-proton Coulomb transition matrix and the free resolvent that indeed do not coincide in the expression for the elastic amplitude. However, they apparently missed the fact that the off-shell proton-proton transition matrix, though exists in the unscreened limit without renormalization, nevertheless carries the singularity of the Coulomb potential, which together with the deuteron pole leads to coinciding singularities in proton-deuteron scattering equations. For example, the analysis of the off-shell t_c^R in the unscreened limit of Eq. (D.8) of Ref. [5] reveals that this takes place for $|\mathbf{p} \pm \mathbf{q}/2| = q_0$, in combination with P leading to the appearance of coinciding singularities of type (9) in (D.9), that are not taken into account in the investigation of the unscreened limit. Recently, a statement has been made [11] that those singularities cancel, however, without any proof. By neglecting this type of singularities Witała *et al.* arrived at an erroneous conclusion that the proton-deuteron elastic scattering amplitude in the unscreened limit should exist without renormalization. Noteworthy, the numerical studies of Ref. [5] omitted the term $\langle \phi_d \mathbf{q}_f | Pt_c^R PG_0T | \phi_d \mathbf{q}_i \rangle$, which in the present work is taken as an example for the appearance of coinciding singularities in the $R \to \infty$ limit. The remaining terms in the elastic amplitude of Ref. [5] may cancel partially, possibly reducing the sensitivity of the phase at finite R, since the low-order terms, such as the first and second term in Eq. (13), taken separately do not acquire the diverging phase. The shortcoming of Ref. [5] persists also in subsequent studies of the breakup reaction, and also in a recent preprint [10]. The latter work mostly deals with the decomposition into contributions of low partial waves and the remaining three-dimensional (3D) ones and partial cancellations between them. Considerations of the present work are performed directly in three dimensions, which is more transparent for the analysis of singularities. The practical calculations [4,12] solve the AGS equations at finite screening radius in the angular-momentum representation with a high number of partial waves, much higher than in calculations of Refs. [5,10], such that the additional 3D terms of Ref. [10] become entirely negligible. Finally, the numerical studies [12,13] using full amplitudes clearly confirmed the need for the renormalization of the scattering amplitudes consistently with Refs. [2,4].

The overall phase of the amplitude is irrelevant for observables, but is decisive for phase shifts. A benchmark calculation for the proton-deuteron elastic scattering observables and phase parameters was performed in Ref. [14], comparing momentum-space [4] and coordinate-space [15] results. The necessity for the amplitude renormalization in the unscreened limit is related to the coordinate-space wave function asymptotics, where the phase shifts with respect to Bessel functions have no limit, but do exist with respect to Coulomb functions [16]. The benchmark [14] demonstrated a good agreement between the two methods, further reinforcing the screening and renormalization method. As the benchmarks are important in establishing the validity and accuracy of new techniques, phase shifts should be calculated also using the method of Refs. [5,10]. However, the existence of the unscreened limit for the proton-deuteron amplitude without renormalization claimed in Refs. [5,10] is consistent with existence of standard phase shifts with respect to Bessel functions, but not with Coulomb ones.

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