Scattering theory for arbitrary potentials

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The fundamental quantities of potential scattering theory are generalized to accommodate long-range interactions. Definitions for the scattering amplitude and wave operators valid for arbitrary interactions including potentials with a Coulomb tail are presented. It is shown that for the Coulomb potential the generalized amplitude gives the physical on-shell amplitude without recourse to a renormalization procedure.

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I. INTRODUCTION

The two-body scattering problem is a central subject of quantum mechanics. It is well known that conventional quantum collision theory is formally valid only when the particles interact via short-range potentials (see, e.g., [1]). In the time-dependent formulation, formal scattering theory can be made to include Coulomb long-range potentials by choosing appropriately modified time evolution operators [2,3]. This is equivalent to choosing various forms of renormalization methods [4–9] in the time-independent formulation.

Though the renormalization theories lead to the correct cross sections for the two-body problem, the results from these procedures cannot be regarded as completely satisfactory. For instance, in screening-based renormalization methods [4,7] different ways of shielding lead to different asymptotic forms for the scattering wave function. Generally, these asymptotic forms differ from the physical one obtained from the solution of the Schrödinger equation [10]. The weakest point about these methods, however, is that they give rise to a scattering amplitude that does not exist on the energy shell. This is because the amplitude obtained in these methods has complex factors which are divergent on the energy shell [7,11–15]. These factors, usually containing branch point singularities, must be removed (renormalized) before approaching the on-shell point. Furthermore, the renormalization factors depend on the way the limits are taken when the on-shell point is approached. Thus, the *ad hoc* renormalization procedure is based on prior knowledge of the exact answer to compare with and has no *ab initio* theoretical justification. These issues are discussed in detail in the comprehensive coverage of the subject given by van Haeringen [10].

The motivation for the present work is to demonstrate that there is a practical approach to the two-body collision problem with a Coulomb-like potential that does not lead to the formal difficulties described above. Our approach is based on a representation of the scattering amplitude written in a divergence-free surface-integral form which is ideally suited for practical calculations. We build on a recent formalism which has improved our understanding of the three-body scattering processes [16,17]. In this work we consider Coulomb-like local long-range potentials. However, their short-range parts can be both local and non-local. One may expect that the method developed here will be useful for potentials with non-local long-range tails as well.

In Sec. II we present a formal solution of the Schrödinger equation which satisfies all necessary conditions imposed by the long-range nature of the Coulomb interaction. We introduce well-defined forms of the scattering amplitude and wave operators for two-body systems valid for arbitrary interactions. The generalized definitions of the scattering amplitude not only cover arbitrary potentials but also directly give the physical result. The relationship with conventional formulations is discussed in Sec. III. Section IV contains some concluding remarks including a brief discussion of the utility of the two-body formalism for three-body Coulomb scattering problems above the breakup threshold.

II. FORMALISM FOR LONG-RANGE POTENTIALS

We consider scattering in a system of two particles 1 and 2 interacting via an arbitrary spherically symmetric potential V with the Coulomb long-range tail. Throughout the paper we use such units that $\hbar=1$. A scattering state of this system is the solution to the Schrödinger equation

$$(E-H)\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})=0, \qquad (1)$$

where $H=H_0+V$ is the total two-body Hamiltonian of the system, $H_0=-\Delta_r/2\mu$ is the free Hamiltonian, $E=k^2/2\mu$ is the energy of the system, $\boldsymbol{r}$ is the relative coordinate of the particles 1 and 2 and $\boldsymbol{k}$ is their relative momentum, and μ is their reduced mass. To be more specific we can assume that interaction V consists of some short-range part V_s and the Coulomb potential $V_c=z_1z_2/r$, where z_1 and z_2 are the charges of the particles.

From all possible solutions to Eq. (1) we should choose the one satisfying the asymptotic boundary condition corresponding to the physical scattering picture. When the poten

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tial has the Coulomb tail the scattering wave function $\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ asymptotically behaves, in the leading order, like the Coulomb-modified plane wave and a Coulomb-modified outgoing spherical wave:

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) \underset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\gamma\ln(kr-\boldsymbol{k}\cdot\boldsymbol{r})}[1+O(1/r)] + f(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}})\frac{e^{ikr-i\gamma\ln(2kr)}}{r}[1+O(1/r)], \tag{2}$$

where $\gamma=z_1z_2\mu/k$ and f is the scattering amplitude. The second suitable solution $\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r})$ asymptotically behaves, in the leading order, like the Coulomb-modified plane wave and a Coulomb-modified incoming spherical wave:

$$\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r}) \underset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}-i\gamma\ln(kr+\boldsymbol{k}\cdot\boldsymbol{r})}[1+O(1/r)] + f^{*}(-\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}})\frac{e^{-ikr+i\gamma\ln(2kr)}}{r}[1+O(1/r)]. \tag{3}$$

Note that $\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}\neq\pm1$, respectively, for Eqs. (2) and (3). However, as we will see below, in the asymptotic sense for which Eqs. (2) and (3) are written these forward-backward singularities have a δ-function nature and are, therefore, integrable. We will also see that seemingly different forms of the Coulomb-modified plane wave in Eqs. (2) and (3) asymptotically are essentially the same function.

We can separate $\psi_{\boldsymbol{k}}^{\pm}$ into the so-called "incident" and "scattered" parts according to

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) + \chi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}), \tag{4}$$

where $\phi_{\boldsymbol{k}}^{\pm}$ and $\chi_{\boldsymbol{k}}^{\pm}$ asymptotically behave like the first and second terms of Eqs. (2) and (3), respectively. The "unscattered" wave incident at infinitely large distances is given by [10]

$$\phi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}\pm i\gamma\ln(kr\mp\boldsymbol{k}\cdot\boldsymbol{r})}\sum_{n=0}^{\infty}[(\mp i\gamma)_n]^2(\mp ikr+i\boldsymbol{k}\cdot\boldsymbol{r})^{-n}/n!, \tag{5}$$

where $(z)_n=z(z+1)\cdots(z+n-1)$. As to the unknown scattered wave $\chi_{\boldsymbol{k}}^{\pm}$, the form of Eqs. (2) and (3) suggests that its leading-order term in the asymptotic region already contains all the scattering information we want. The next-order terms simply repeat this information. Therefore, all we need for extracting the scattering amplitude is the leading-order asymptotic term of the scattered wave $\chi_{\boldsymbol{k}}^{\pm}$.

Let us denote $\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})$ the first term of the incident wave $\phi_{\boldsymbol{k}}^{\pm}$,

$$\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}\pm i\gamma\ln(kr\mp\boldsymbol{k}\cdot\boldsymbol{r})}, \tag{6}$$

and by $\phi_{\boldsymbol{k}}^{(1)\pm}(\boldsymbol{r})$ the second term, etc.:

$$\phi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}) + \phi_{\boldsymbol{k}}^{(1)\pm}(\boldsymbol{r}) + \phi_{\boldsymbol{k}}^{(2)\pm}(\boldsymbol{r}) + \cdots. \tag{7}$$

Then Eq. (1) can be written in the form

$$(E-H)[\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) - \phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})] = (H-E)\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}). \tag{8}$$

If we introduce Green's function according to

$$(E-H)G(\boldsymbol{r},\boldsymbol{r}',E) = \delta(\boldsymbol{r}-\boldsymbol{r}') \tag{9}$$

and apply it onto both sides of Eq. (8), we have

$$\int d\boldsymbol{r}'\, G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)(E-\vec{H})[\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}') - \phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}')] = \int d\boldsymbol{r}'\, G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)(\vec{H}-E)\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}'), \tag{10}$$

where ϵ is a small positive parameter and a limit as $\epsilon\to0$ is assumed [18]. We used an arrow on the differential Hamiltonian operator to show the direction in which it acts. We emphasize here a subtle point that the operator $G(\boldsymbol{r},\boldsymbol{r}',E)(E-\vec{H})$ in Eq. (10) does not act like a δ function. In other words, though

$$G(\boldsymbol{r},\boldsymbol{r}',E)(E-\overleftarrow{H}) = (E-\vec{H})G(\boldsymbol{r},\boldsymbol{r}',E) \equiv \delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{11}$$

however, in general,

$$G(\boldsymbol{r},\boldsymbol{r}',E)(E-\vec{H}) \neq \delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{12}$$

The reason is that the operator $G(\boldsymbol{r},\boldsymbol{r}',E)(E-\vec{H})$ produces an integral that has a surface-integral component. In order for the action of the operator $G(\boldsymbol{r},\boldsymbol{r}',E)(E-\vec{H})$ to be equal to that of $G(\boldsymbol{r},\boldsymbol{r}',E)(E-\overleftarrow{H})$ this surface-integral component should be zero. A similar problem has been discussed by Glöckle [19] in relation to the three-body Lippmann-Schwinger equations. Using an operator similar to ours but with the Hamiltonian H and the Green's function G replaced by some channel Hamiltonian and corresponding Green's function Glöckle showed that surface integrals of the same nature only disappear if the operator acts on a function which vanishes sufficiently quickly at infinity. It is not difficult to demonstrate that the same conclusion also applies to operator $G(\boldsymbol{r},\boldsymbol{r}',E)(E-\vec{H})$. Since the wave functions $\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})-\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})$ and $\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})$ are examples of functions which do not vanish at infinity the surface integral terms generated do not vanish.

On the right-hand side of Eq. (10) we have a purely scattered wave generated from $\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})$. Therefore, we denote the result of the action of the integral operator on the left-hand side of Eq. (10) as

$$\int d\boldsymbol{r}'\, G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)(E-\vec{H})[\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) - \phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})] \equiv \chi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}), \tag{13}$$

which is a part of the scattered wave $\chi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})$. Then, for the part of the total scattering wave function $\psi_{\boldsymbol{k}}^{(0)\pm}$ developed from the leading term of the incident wave,

$$\psi_{\boldsymbol{k}}^{(0)\pm} \equiv \phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}) + \chi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}), \tag{14}$$

we can write

$$\psi_k^{(0)\pm}(r) = \phi_k^{(0)\pm}(r) + \int dr' G(r,r';E \pm i\epsilon)(\vec{H} - E)\phi_k^{(0)\pm}(r'). \tag{15}$$

Note that although $\phi_k^{(0)\pm}(r)$ is just the leading-order term of the incident wave, $\psi_k^{(0)\pm}(r)$ includes scattered waves of all orders through the Green's function. Moreover, as we will see below the scattered wave in Eq. (15) is in fact the only scattered part of the total wave function $\psi_k^{\pm}(r)$.

Similarly, if $\phi_k^{(1)\pm}$ is the next-to-the-leading-order term of the incident wave, then

$$(E - H)[\psi_k^{\pm}(r) - \phi_k^{(1)\pm}(r)] = (H - E)\phi_k^{(1)\pm}(r). \tag{16}$$

Therefore, for the part of the scattering wave $\psi_k^{\pm}$ developed from the $\phi_k^{(1)\pm}$ term [i.e., for $\psi_k^{(1)\pm} \equiv \phi_k^{(1)\pm}(r) + \chi_k^{(1)\pm}(r)$] we have

$$\psi_k^{(1)\pm}(r) = \phi_k^{(1)\pm}(r) + \int dr' G(r,r';E \pm i\epsilon)(\vec{H} - E)\phi_k^{(1)\pm}(r'). \tag{17}$$

By direct substitution of Eqs. (15) and (17) into Eq. (1) and using Eq. (9) we verify that $\psi_k^{(0)\pm}(r)$ and $\psi_k^{(1)\pm}(r)$ satisfy Eq. (1). Obviously, continuing this procedure $\psi_k^{\pm}(r)$ can be formally reconstructed:

$$\psi_k^{\pm}(r) = \psi_k^{(0)\pm}(r) + \psi_k^{(1)\pm}(r) + \psi_k^{(2)\pm}(r) + \cdots. \tag{18}$$

The latter can simply be written as

$$\psi_k^{\pm}(r) = \phi_k^{\pm}(r) + \int dr' G(r,r';E \pm i\epsilon)(\vec{H} - E)\phi_k^{\pm}(r'). \tag{19}$$

It is easily verified (by substitution) that this is a formal solution to Eq. (1). Generally, this solution is not unique. The physical solution is the one which satisfies the boundary conditions specified in Eq. (2) or (3). At first sight the integral term in Eq. (19) seems to involve a nonintegrable singularity at the origin for the higher-order terms of the incident wave. However, as we will now demonstrate, this is not the case.

We begin by noting as mentioned earlier that the leading-order asymptotic term of $\psi_k^{\pm}(r)$ already contains all the scattering information we need, provided Eq. (19) is the solution which has the required asymptotic behavior. In other words, for the purpose of extracting the scattering amplitude we have to verify that Eq. (19) asymptotically behaves as Eq. (2) or (3). To this end let us write the full set of eigenstates of Hamiltonian H as $\{\psi_k^{\pm}, \varphi_n\}$, where φ_n are the eigenfunctions corresponding to negative discrete eigenvalues E_n. Then we express the Green's function in its spectral decomposition as

$$G(r,r';E \pm i\epsilon) = \int \frac{dk'}{(2\pi)^3} \frac{\psi_{k'}^{\mp}(r)\psi_{k'}^{\mp *}(r')}{E - k'^2/2\mu \pm i\epsilon} + \sum_n \frac{\varphi_n(r)\varphi_n^*(r')}{E - E_n \pm i\epsilon}. \tag{20}$$

Using this we can write Eq. (19) as

$$\psi_k^{+}(r) = \phi_k^{+}(r) + \int \frac{dk'}{(2\pi)^3} \frac{\langle \psi_{k'}^{-}|\vec{H} - E|\phi_k^{+}\rangle \psi_{k'}^{-}(r)}{E - k'^2/2\mu + i\epsilon} + \cdots, \tag{21}$$

where the ellipsis indicates the contribution from the bound states. As we are interested only in the asymptotic behavior when $r \to \infty$ the bound states do not contribute.

Consider now

$$\langle \psi_{k'}^{-}|\vec{H} - E|\phi_k^{+}\rangle \equiv \int dr\, \psi_{k'}^{-*}(r)(\vec{H} - E)\phi_k^{+}(r), \tag{22}$$

the integral entering Eq. (21). This is a kind of integral with a possible nonvanishing surface-integral component we mentioned earlier. Using Eq. (1) we can write

$$\begin{aligned}\langle \psi_{k'}^{-}|\vec{H} - E|\phi_k^{+}\rangle &= \langle \psi_{k'}^{-}| - \overleftarrow{H} + E + \vec{H} - E|\phi_k^{+}\rangle \\ &= -\langle \psi_{k'}^{-}|\overleftarrow{H}_0 - \vec{H}_0|\phi_k^{+}\rangle.\end{aligned} \tag{23}$$

Using Green's theorem this volume integral can be transformed to a surface integral. We have

$$\begin{aligned}\langle \psi_{k'}^{-}|\vec{H} - E|\phi_k^{+}\rangle &= -\frac{1}{2\mu}\lim_{r\to\infty} r^2 \int \hat{r}\, d\hat{r}[\psi_{k'}^{-*}\nabla_r\phi_k^{+} - \phi_k^{+}\nabla_r\psi_{k'}^{-*}] \\ &= -\frac{1}{2\mu}\lim_{r\to\infty} r^2 \int d\hat{r}\left[\psi_{k'}^{-*}\frac{\partial\phi_k^{+}}{\partial r} - \phi_k^{+}\frac{\partial\psi_{k'}^{-*}}{\partial r}\right].\end{aligned} \tag{24}$$

Thus in the surface-integral form our integral depends only on the asymptotic behavior of the participating functions. Now noting that

$$\phi_k^{\pm}(r) \underset{r\to\infty}{\sim} \phi_k^{(0)\pm}(r)[1 + O(1/r)], \tag{25}$$

it is easy to see that

$$\langle \psi_{k'}^{-}|\vec{H} - E|\phi_k^{+}\rangle = -\langle \psi_{k'}^{-}|\overleftarrow{H}_0 - \vec{H}_0|\phi_k^{(0)+}\rangle = \langle \psi_{k'}^{-}|\vec{H} - E|\phi_k^{(0)+}\rangle. \tag{26}$$

In combination with Eq. (21) this result in fact means that

$$\begin{aligned}&\int dr' G(r,r';E \pm i\epsilon)(\vec{H} - E)\phi_k^{\pm}(r') \\ &\quad = \int dr' G(r,r';E \pm i\epsilon)(\vec{H} - E)\phi_k^{(0)\pm}(r');\end{aligned} \tag{27}$$

i.e., all the scattered wave is generated from the first term of the incident wave $\phi_k^{(0)+}$. In other words, somewhat unexpectedly, no scattered wave is produced from the remaining part of ϕ_k^{+}. This also shows that Eq. (19) does not contain nonintegrable singularities for small r'.

Thus, using Eq. (26) we can write Eq. (21) as

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = \phi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) + \int \frac{d\boldsymbol{k}'}{(2\pi)^3}\frac{T(\boldsymbol{k}',\boldsymbol{k})\psi_{\boldsymbol{k}'}^{-}(\boldsymbol{r})}{E - k'^2/2\mu + i\epsilon} + \cdots, \quad (28)$$

where the ellipsis still indicates only the contribution from the bound states. In the above equation we have introduced the notation

$$T(\boldsymbol{k}',\boldsymbol{k}) = \langle \psi_{\boldsymbol{k}'}^{-}|\vec{H} - E|\phi_{\boldsymbol{k}}^{(0)+}\rangle, \quad (29)$$

anticipating that $T(\boldsymbol{k}',\boldsymbol{k})$ is the desired scattering T matrix. However, this requires justification, which we now provide. In order to prove this let us first expand the scattering wave function $\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$ according to

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) = \sum_{l,m} i^l e^{i\sigma_l(k)}\chi_l(k,r)Y_{l,m}^{*}(\hat{\boldsymbol{k}})Y_{l,m}(\hat{\boldsymbol{r}}), \quad (30)$$

where $\sigma_l(k)$ is the (total) phase shift. The radial functions asymptotically behave according to

$$\chi_l(k,r) \underset{r\to\infty}{\sim} \frac{4\pi}{kr}\sin[kr - \gamma\ln|2kr| - l\pi/2 + \sigma_l(k)]. \quad (31)$$

Therefore, substituting Eq. (31) into Eq. (30) we get, after some algebra,

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) \underset{r\to\infty}{\sim} \frac{2\pi}{ikr}[e^{ikr-i\gamma\ln|2kr|}\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}}) - e^{-ikr+i\gamma\ln|2kr|}\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})] + \frac{e^{ikr-i\gamma\ln|2kr|}}{r}\frac{2\pi}{ik}\sum_{l,m}(e^{2i\sigma_l(k)}-1)Y_{l,m}^{*}(\hat{\boldsymbol{k}})Y_{l,m}(\hat{\boldsymbol{r}}). \quad (32)$$

Since [20]

$$\frac{2\pi}{ik}\sum_{l,m}(e^{2i\sigma_l(k)}-1)Y_{l,m}^{*}(\hat{\boldsymbol{k}})Y_{l,m}(\hat{\boldsymbol{r}}) = f(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}), \quad (33)$$

we may conclude that Eq. (32) is equivalent to Eq. (2). The amplitude f is still unknown; however, from here we get an interesting result that the first term of Eq. (32) is an asymptotic form of the distorted plane wave $\phi_{\boldsymbol{k}}^{(0)+}(\boldsymbol{r})$. Repeating the same reasoning for $\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r})$ [or using $\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r}) = \psi_{-\boldsymbol{k}}^{+*}(\boldsymbol{r})$] we establish that exactly the same term is the asymptotic form of $\phi_{\boldsymbol{k}}^{(0)-}(\boldsymbol{r})$ as well. That is,

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}\pm i\gamma\ln(kr\mp\boldsymbol{k}\cdot\boldsymbol{r})} \underset{r\to\infty}{\sim} \frac{2\pi}{ikr}[e^{ikr-i\gamma\ln|2kr|}\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}}) - e^{-ikr+i\gamma\ln|2kr|}\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})]. \quad (34)$$

In the absence of long-range distortion, Eq. (34) transforms to the familiar asymptotic form of the plane wave (see, e.g., Ref. [22]):

$$e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \underset{r\to\infty}{\sim} \frac{2\pi}{ikr}[e^{ikr}\delta(\hat{\boldsymbol{k}}-\hat{\boldsymbol{r}}) - e^{-ikr}\delta(\hat{\boldsymbol{k}}+\hat{\boldsymbol{r}})]. \quad (35)$$

Thus the beauty of the result is that the notorious forward-backward singularity of the distorted plane waves $\phi_{\boldsymbol{k}}^{(0)+}(\boldsymbol{r})/\phi_{\boldsymbol{k}}^{(0)-}(\boldsymbol{r})$ is shown to be no more problematic than a δ function. Therefore, in the asymptotic region the distorted plane wave can be treated much like the plane wave. In this regard it is worth mentioning that the Coulomb Green's function in momentum space has also been shown to have distorted pole singularities [23] which follow from the existence of the Dollard wave operators.

Returning to Eq. (28) we have asymptotically, in the leading order,

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) \underset{r\to\infty}{\sim} \phi_{\boldsymbol{k}}^{(0)+}(\boldsymbol{r}) + \int \frac{d\boldsymbol{k}'}{(2\pi)^3}\frac{T(\boldsymbol{k}',\boldsymbol{k})\phi_{\boldsymbol{k}'}^{(0)-}(\boldsymbol{r})}{E - k'^2/2\mu + i\epsilon}. \quad (36)$$

When $r\to\infty$ the components involving bound states decrease exponentially. Thus we have the two-body version of the asymptotic relationship revealed in Refs. [24,25]. It states that the leading-order asymptotic term of the scattering wave is defined by the same (i.e., the leading-order) asymptotic term of the incident wave. Using Eq. (34) and evaluating the integral, taking advantage of the simple pole singularity of the integrand at the on-shell point [26], we have

$$\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r}) \underset{r\to\infty}{\sim} e^{i\boldsymbol{k}\cdot\boldsymbol{r}+i\gamma\ln(kr-\boldsymbol{k}\cdot\boldsymbol{r})} - \frac{\mu}{2\pi}T(k\hat{\boldsymbol{r}},\boldsymbol{k})\frac{e^{ikr}}{r}e^{-i\gamma\ln(2kr)}. \quad (37)$$

In Eq. (37) we dropped the modulus sign since at this stage it is safe to do so. By comparing Eqs. (37) and (2) we conclude, as we set out to prove, that $T(\boldsymbol{k}',\boldsymbol{k})$ introduced in Eq. (29) is the transition matrix (T matrix) which defines the amplitude of scattering of the particles with initial relative momentum $\boldsymbol{k}$ in the direction of $\boldsymbol{r}$:

$$f(\hat{\boldsymbol{k}}\cdot\hat{\boldsymbol{r}}) = -\frac{\mu}{2\pi}T(\boldsymbol{k}',\boldsymbol{k}), \quad (38)$$

where we used a notation $\boldsymbol{k}' = k\hat{\boldsymbol{r}}$. In analogy with conventional scattering theory we call the new form for $T(\boldsymbol{k}',\boldsymbol{k})$ as defined in Eq. (29) the *prior* form of the T matrix.

Repeating the procedure outlined above for $\psi_{\boldsymbol{k}}^{-}(\boldsymbol{r})$ [this time we use the resolution of the total Green's function G in terms of $\psi_{\boldsymbol{k}}^{+}(\boldsymbol{r})$] we get

$$T^{post}(\boldsymbol{k}',\boldsymbol{k}) = \langle \phi_{\boldsymbol{k}'}^{(0)-}|\overleftarrow{H} - E|\psi_{\boldsymbol{k}}^{+}\rangle. \quad (39)$$

In obtaining Eq. (39) we also used the reciprocity theorem—i.e., $T(\boldsymbol{k}',\boldsymbol{k}) = T(-\boldsymbol{k},-\boldsymbol{k}')$ [27]. Again, in analogy with the standard theory this new form is called the *post* form of the T matrix.

In deriving the result of Eq. (26) we saw, in particular, that

$$T^{prior}(\boldsymbol{k}',\boldsymbol{k}) = -\langle \psi_{\boldsymbol{k}'}^{-}|\overleftarrow{H}_0 - \vec{H}_0|\phi_{\boldsymbol{k}}^{(0)+}\rangle, \quad (40)$$

$$= -\frac{1}{2\mu}\lim_{r\to\infty} r^2\int d\hat{\boldsymbol{r}}\left[\psi_{\boldsymbol{k}'}^{-*}\frac{\partial\phi_{\boldsymbol{k}}^{(0)+}}{\partial r} - \phi_{\boldsymbol{k}}^{(0)+}\frac{\partial\psi_{\boldsymbol{k}'}^{-*}}{\partial r}\right]. \quad (41)$$

In a similar way we also get, from Eq. (39),

$$T^{post}(\boldsymbol{k}',\boldsymbol{k}) = \langle \phi_{\boldsymbol{k}'}^{(0)-}|\overleftarrow{H}_0 - \vec{H}_0|\psi_{\boldsymbol{k}}^{+}\rangle. \quad (42)$$

$$=\frac{1}{2\mu}\lim_{r\to\infty} r^2 \int d\hat{\boldsymbol{r}}\left[\phi_{\boldsymbol{k}'}^{(0)-*}\frac{\partial\psi_{\boldsymbol{k}}^{+}}{\partial r}-\psi_{\boldsymbol{k}}^{+}\frac{\partial\phi_{\boldsymbol{k}'}^{(0)-*}}{\partial r}\right]. \quad (43)$$

Thus the scattering T matrix conventionally given as volume integrals can be written equivalently in surface-integral forms. We emphasize that in these forms the T matrix depends only on the asymptotic behavior of the participating functions. Therefore, knowledge of the scattering wave function over the entire space is not required. In addition, the surface-integral forms are readily expanded in partial waves, leading to a simple analytic result containing only the limiting procedure. Therefore, these forms are particularly suitable for practical calculations. It is also interesting to note the close resemblance of these forms to the representation of the number of scattered particles crossing the surface element $d\hat{\boldsymbol{r}}$ per unit time at large distance r. In that sense, the surface-integral forms further reveal the scattering amplitude as the amplitude of the probability flux of particles scattered in direction $\hat{\boldsymbol{r}}$.

We note that in an operator form Eq. (19) can be written as

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})=[1+G(E\pm i\epsilon)(\vec{H}-E)]\phi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}), \quad (44)$$

where $G(E\pm i\epsilon)=(E\pm i\epsilon-H)^{-1}$ is the Green's operator associated with the Green's function $G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)$. Therefore, we can introduce new generalized wave operators according to

$$\Omega^{\pm}=[1+G(E\pm i\epsilon)(\vec{H}-E)]. \quad (45)$$

In the next section we turn to a further investigation of these generalized wave operators.

III. CONSISTENCY WITH CONVENTIONAL RESULTS

Our aim in this section is to show the results given above are consistent with conventional potential scattering theory for short-range interactions. The existing formulation of scattering theory relies on the condition that interaction $V(r)$ decreases faster than the Coulomb interaction when $r\to\infty$ [$\gamma=0$ in Eqs. (5) and (6)], so that

$$\phi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})=\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})\to\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})=e^{i\boldsymbol{k}\cdot\boldsymbol{r}}. \quad (46)$$

The initial unscattered wave function satisfies the Helmholtz equation

$$(E-H_0)\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})=0. \quad (47)$$

Then,

$$(H-E)\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})=V\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r}); \quad (48)$$

therefore, Eq. (19) takes the form

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})=\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})+\int d\boldsymbol{r}'\,G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)(\vec{H}-E)\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r}')$$

$$=\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r})+\int d\boldsymbol{r}'\,G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)V\phi_{\boldsymbol{k}}^{(0)}(\boldsymbol{r}'). \quad (49)$$

This is the formal solution which is obtained in conventional scattering theory. In the light of Eq. (48), Eqs. (29) and (39) reduce to

$$T^{prior}(\boldsymbol{k}',\boldsymbol{k})=\langle\psi_{\boldsymbol{k}'}^{-}|V|\phi_{\boldsymbol{k}}^{(0)}\rangle, \quad (50)$$

$$T^{post}(\boldsymbol{k}',\boldsymbol{k})=\langle\phi_{\boldsymbol{k}'}^{(0)}|V|\psi_{\boldsymbol{k}}^{+}\rangle, \quad (51)$$

in agreement with the standard definitions of the T matrix. Moreover, for the same reason the generalized wave operators $\Omega^{\pm}$ introduced above reduce to the usual Möller (M) ones:

$$\Omega_{\mathrm{M}}^{\pm}=[1+G(E\pm i\epsilon)V]. \quad (52)$$

Obviously, when interaction V has a tail which does not disappear at infinity, the Helmholtz equation (47) for $\phi_{\boldsymbol{k}}^{(0)+}$ and, consequently, Eq. (48) are not satisfied. As a result Eqs. (49)–(51) are incorrect and Eq. (52) is not valid for Coulomb-like potentials.

On the other hand, when the interaction is purely Coulomb, we can proceed further with analytical methods. Then we have

$$(H-E)\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})=\frac{\gamma^2 k}{\mu r(kr\mp\boldsymbol{k}\cdot\boldsymbol{r})}\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}). \quad (53)$$

Therefore, Eqs. (29) and (39) transform to

$$T^{prior}(\boldsymbol{k}',\boldsymbol{k})=\left\langle\psi_{\boldsymbol{k}'}^{-}\left|\frac{\gamma^2 k}{\mu r(kr-\boldsymbol{k}\cdot\boldsymbol{r})}\right|\phi_{\boldsymbol{k}}^{(0)+}\right\rangle, \quad (54)$$

$$T^{post}(\boldsymbol{k}',\boldsymbol{k})=\left\langle\phi_{\boldsymbol{k}'}^{(0)-}\left|\frac{\gamma^2 k}{\mu r(kr+\boldsymbol{k}\cdot\boldsymbol{r})}\right|\psi_{\boldsymbol{k}}^{+}\right\rangle. \quad (55)$$

Here $\psi_{\boldsymbol{k}}^{\pm}$ are known and given by

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})=e^{i\boldsymbol{k}\cdot\boldsymbol{r}}e^{-\pi\gamma/2}\Gamma(1\pm i\gamma)\,{}_1F_1(\mp i\gamma,1,\pm ikr-i\boldsymbol{k}\cdot\boldsymbol{r}), \quad (56)$$

with ${}_1F_1$ being the usual confluent hypergeometric function. At the same time Eq. (15) transforms to

$$\psi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})=\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})+\int d\boldsymbol{r}'\,G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)$$

$$\times\frac{\gamma^2 k}{\mu r'(kr'\mp\boldsymbol{k}\cdot\boldsymbol{r}')}\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}'). \quad (57)$$

This is to be compared with the result obtained in Eq. 16 of Ref. [28] for the total scattering wave function $\psi_{\boldsymbol{k}}^{\pm}$:

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})=\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r})+\int d\boldsymbol{r}'\,G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)$$

$$\times\frac{\gamma^2 k}{\mu r'(kr'\mp\boldsymbol{k}\cdot\boldsymbol{r}')}\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}'). \quad (58)$$

If Eq. (58) were true, it would mean that

$$\int d\boldsymbol{r}'\,G(\boldsymbol{r},\boldsymbol{r}';E\pm i\epsilon)(E-\vec{H})[\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}')-\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}')]$$

$$=\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})-\phi_{\boldsymbol{k}}^{(0)\pm}(\boldsymbol{r}), \quad (59)$$

which is, however, not correct [see Eq. (10) and the discussion following it]. Based on Eq. (58) Barrachina and Macek also arrived at Eq. (55); nevertheless, since the underlying equation was not correct, this result is not justified in Ref. [28]. On a positive note, the matrix elements in Eqs. (54) and (55) (to be more precise, the complex conjugate of the former) have been evaluated in Ref. [28] in closed form. We have checked and confirm their result—namely,

$$\left\langle \psi_{\boldsymbol{k}'}^{-} \left| \frac{\gamma^2 k}{\mu r(kr - \boldsymbol{k}\cdot\boldsymbol{r})} \right| \phi_{\boldsymbol{k}}^{(0)+} \right\rangle \equiv \left\langle \phi_{\boldsymbol{k}'}^{(0)-} \left| \frac{\gamma^2 k}{\mu r(kr + \boldsymbol{k}\cdot\boldsymbol{r})} \right| \psi_{\boldsymbol{k}}^{+} \right\rangle = \frac{4\pi z_1 z_2}{|\boldsymbol{k}'-\boldsymbol{k}|^2}\frac{\Gamma(1+i\gamma)}{\Gamma(1-i\gamma)}\left[\frac{4k^2}{|\boldsymbol{k}'-\boldsymbol{k}|^2}\right]^{i\gamma}, \tag{60}$$

which is the well-known full on-shell Coulomb T matrix. This gives additional support for the new definitions of the T matrix.

Finally, in the pure Coulomb case the generalized wave operators $\Omega^{\pm}$ introduced earlier reduce to the wave operators obtained by Mulherin and Zinnes (MZ) [29]:

$$\Omega_{\mathrm{MZ}}^{\pm} = \left[1 + G(E \pm i\epsilon)\frac{\gamma^2 k}{\mu r(kr \mp \boldsymbol{k}\cdot\boldsymbol{r})} \right], \tag{61}$$

provided $\Omega^{\pm}$ are applied to the first term of the incident wave $\phi_{\boldsymbol{k}}^{(0)\pm}$. This clearly shows that the MZ operators are approximations to the corresponding full wave operators. Obviously, this approximation makes a sense only for asymptotically large distances where $\phi_{\boldsymbol{k}}^{(0)\pm}$ becomes the dominant (leading-order) term. Elsewhere, the MZ operator cannot be relied upon. This finding may also explain formal problems associated with the MZ approach [30].

IV. CONCLUSION

In this paper we have presented a generalization of potential scattering theory which is valid for arbitrary interactions including potentials with the long-range Coulomb tail. We obtained a formal solution to the Schrödinger equation satisfying the boundary conditions imposed by the long-range nature of the Coulomb interaction. We introduced general definitions for the scattering amplitude and wave operators. We showed that when the interaction potential is short ranged the generalized definitions of the scattering amplitude and wave operators transform to the conventional ones used in standard scattering theory. A distinctly satisfying feature of the presented forms for the scattering amplitude is that they do not contain divergent factors and directly give the physical on-shell scattering amplitude even when the interaction potential is long ranged. Moreover, the generalized wave operators are also the same for arbitrary potentials including the long-range interactions. Therefore, no modification of the theory based on renormalization is required. The results of the present work close the gap between the two different formulations of potential scattering theory for short- and long-range interactions.

In conclusion we make the following comments. In the literature devoted to the Coulomb scattering it is customary to separate $\psi_{\boldsymbol{k}}^{\pm}$ into the "incident" and "scattered" parts according to

$$\psi_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = \tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) + \tilde{\chi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}), \tag{62}$$

where the incident wave is taken as [10]

$$\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = e^{i\boldsymbol{k}\cdot\boldsymbol{r}} e^{\pi\gamma/2} U(\mp i\gamma, 1, \pm ikr - i\boldsymbol{k}\cdot\boldsymbol{r}). \tag{63}$$

Here U is the confluent hypergeometric function of the second kind. The idea is driven by the fact that the confluent hypergeometric function in the regular Coulomb function [see Eq. (56)] can be written as a sum of two irregular confluent hypergeometric functions of the second kind and that functions $\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})$ and $\tilde{\chi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})$ satisfy the first and second parts of asymptotic condition (2) or (3), respectively. However, (for the pure Coulomb interaction) $\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r})$ alone is a solution to the original Schrödinger equation: i.e.,

$$(E - H)\tilde{\phi}_{\boldsymbol{k}}^{\pm}(\boldsymbol{r}) = 0. \tag{64}$$

Consequently, the scattered wave $\tilde{\chi}_{\boldsymbol{k}}^{\pm}$ is a solution as well. Thus, as a result of separation (62), Eq. (1) splits into two equations, making it impossible to single out uniquely the important surface-integral components in the full solution. Therefore representation (62) is not a satisfactory starting point. It also leads to other anomalies associated with the Coulomb problem. In particular, using Eq. (64) one can demonstrate that the Coulomb wave function is a solution to a *homogeneous* Lippmann-Schwinger equation [31]. On the other hand, the splitting (4) used in this work represents the logical fact that the "unscattered" incident wave is coming from infinity and should be taken in a form valid at asymptotically large distances.

We conclude by offering a few comments on the possible usefulness of our method for three-body systems with long-range interactions. A rigorous scattering theory for a system of three particles valid for short-range potentials was given by Faddeev [32,33]. For charged particles with the long-range Coulomb interaction the theory has faced apparently insurmountable difficulties. The problem is that the Faddeev equations are not compact in the presence of Coulomb interactions. In other words, these equations cannot be solved using standard numerical procedures. Considerable progress has been made in dealing with aspects of the three-body problem with Coulomb-like potentials. In particular, a renormalization method based on screening [4,7] has been implemented successfully for the case when two particles are charged [34,35]. The method has also been extended to two-fragment reactions in a system of three charged particles [35,36]. However, no practical time-independent renormalization method exists that is valid for a system of three charged particles above the breakup threshold, though Dollard's time-dependent approach [2,3] is formally valid for arbitrary multichannel collisions including three-body problems. The problem is that above the threshold the Coulomb three-body system possesses essentially different types of singularities and the two-particle renormalization procedures are not sufficient to guarantee compactness of the equations [5,37,38]. Thus, on the one hand, there are no integral equations yet known for collisions of more than two charged particles that are satisfactory above the breakup threshold

[10], and on the other hand, there is also neither theoretical proof nor practical evidence that the renormalization approach can be applied to the Faddeev equations for the genuine three-body Coulomb problem. This is a rather disturbing situation especially for the atomic three-body problem where all three particles are charged. Therefore, generally speaking, it would be useful to formulate three-body scattering theory in a manner that does not require renormalization so that the aforementioned modifications are, in a certain sense, unnecessary. We are confident that the method proposed here for solving the two-body problem that was free of the usual Coulomb anomalies can be profitably applied to the proper formulation of the three-body rearrangement theory for long-range interactions.

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