Higher-order poles and mass-shell singularities in electron-hydrogen scattering

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The forward scattering amplitude for electron-hydrogen scattering is expected to be an analytic function of the energy. However, when calculated within the framework of nonrelativistic quantum mechanics and the Born approximation, the exchange part has double and triple left-hand poles. From the viewpoint of field theory, such higher-order singularities are unexpected: One normally encounters only simple poles and branch points. A simple nonrelativistic model, which interpolates between binding by short-range and long-range forces, is used to show that these singularities are a direct consequence of the fact that the target system is bound by Coulomb forces: If the binding is by short-range forces there is only a simple pole. The double and triple poles emerge from a coalescence of simple poles and logarithmic branch points, in the limit of long-range binding. In the same framework, the direct amplitude has both simple and double poles, regarded as a function of the squared momentum transfer. Now even the simple pole is unexpected because the H atom is neutral. Again, the existence of these singularities is shown to be a consequence of Coulomb binding. The singularities are then studied within the framework of field theory. I show that if the H atom is treated as if it were an elementary particle, described by a field ϕ_{H} coupled to electron and proton fields ϕ_e and ϕ_p by a Lagrangian density $L_I = -G_0(\phi_e \phi_p)^\dagger \phi_{\mathrm{H}} + \mathrm{H.c.}$, the location of the singularity of the exchange amplitude is immediately obtained from a tree diagram, without the need to carry out any integrations. However, the nature of the singularity found does not agree with the nonrelativistic theory: There is no free lunch. Further analysis indicates that in full-fledged quantum electrodynamics, the vertex function Γ which describes the virtual decomposition of the H atom into its constituents must itself be singular when all particles are on the mass shell.

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I. INTRODUCTION

The elastic scattering of electrons from hydrogen atoms is one the most basic and venerable problems of atomic physics [1]. Since the problem cannot be solved exactly, even in the framework of nonrelativistic quantum mechanics (NRQM), it has led to much theoretic effort, including work to derive and test dispersion relations (DR) for the forward-scattering amplitude, pioneered by Gerjuoy and Krall [2] and later further developed [3,4]. Recently, there has been renewed interest and progress in the nature of the DR for both the forward and the partial-wave amplitudes [5].

For the application of DR methods, one needs knowledge of the analyticity properties of the scattering amplitude $F = F(\mathbf{k}', \mathbf{k})$, especially the location and nature of its singularities in a complex k^2 plane. With regard to the forward amplitude, $F(k^2) = F(\mathbf{k}, \mathbf{k})$ one expects, by analogy with potential scattering, a branch point at $k^2 = 0$ and a left-hand pole determined by the energy of the weakly bound H^- state. One also expects left-hand singularities arising from exchange. However, from the viewpoint of amplitudes encountered in particle physics there is a surprise in store.

With spin-dependent forces neglected, the amplitude F can be written as a linear combination of a "direct amplitude" f and an "exchange amplitude" g, with $F = f \pm g$, the plus and minus signs corresponding to singlet and triplet initial spin states, respectively. The lowest-order contribution of the electron-electron interaction $V_{12} = e^2/r_{12}$ to g is given by

$$g_{12}^{\mathrm{Born}}(\mathbf{k}', \mathbf{k}) = -(m_e/2\pi\hbar^2)\langle \phi, \mathbf{k}' | e^2/r_{12} | \mathbf{k}, \phi \rangle, \quad (1.1)$$

where $|\mathbf{k}, \phi\rangle = \exp(i\mathbf{k}\cdot\mathbf{r}_1)\phi(\mathbf{r}_2)$, $|\phi, \mathbf{k}'\rangle = \phi(\mathbf{r}_1)\exp(i\mathbf{k}'\cdot\mathbf{r}_2)$, and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$. Here, $\phi(\mathbf{r}_2)$ is the wave function of the H atom in the $1s$ state

$$\phi(\mathbf{r}_2) = (\kappa^3/\pi)^{1/2} \exp(-\kappa r_2), \quad (1.2)$$

where $\kappa = 1/a$ is the inverse of the Bohr radius a. Evaluation of Eq. (1.1) yields, for $\mathbf{k}' = \mathbf{k}$,

$$g_{12}^{\mathrm{Born}}(k^2) = a[c_1(k^2/\kappa^2+1)^{-1} + c_2(k^2/\kappa^2+1)^{-2} + c_3(k^2/\kappa^2+1)^{-3}], \quad (1.3)$$

with $c_1 = -2$, $c_2 = -8/3$, and $c_3 = -16/3$.

The surprise here is the presence of the second- and third-order poles at $k^2 = -\kappa^2$. They are present not only in Born approximation but survive, as one would expect, in analyses which attempt to go beyond this, including the so-called static exchange approximation used by Blum and Burke [3] and the summation of some higher-order exchange effects by Amusia and Kuchiev [4]. (In the literature, the sum $g_1^{\mathrm{Born}} + g_{12}^{\mathrm{Born}}$, where g_1^{Born} is defined by the replacement of e^2/r_{12} by $V_1 = -e^2/r_1$ in Eq. (1.1), is usually called the Born approximation to the exchange amplitude. Discussion of g_1^{Born}, the so-called core term, is deferred to Sec. V.) Another surprise is provided by the direct amplitude in the Born approximation, which has a single and a double pole in the squared momentum transfer; even the single pole is unexpected, because the H atom is neutral.

In the context of particle physics, transition amplitudes can usually be regarded as analytic functions of the relevant variables, such as energy and momentum transfer, with singularities which are either branch points or poles. The physical interpretation of such poles is particularly simple: They correspond to stable particles which the scattering particles can exchange or into which they can (virtually) combine. However, such processes normally lead only to simple poles.

The purpose of this paper is to explain the origin of these singularities within the framework of NRQM and to see what light can be shed on it in the context of relativistic quantum field theory (RQFT). It turns out that there are lessons here for both atomic and particle physics. On the one hand, by regarding the H atom in its ground state as an ordinary, albeit composite, particle, one can understand the existence and location of the singularity from a single Feynman-like diagram, without the need to evaluate any integrals, such as that occuring in Eq. (1.1). On the other hand, analysis of the NRQM calculation reveals that the higher-order poles are solely a consequence of the long-range character of the interaction which binds the target electron to the core proton. This in turn leads to an unexpected conclusion regarding the analytic behavior of the vertex function Γ, which in field theory describes the virtual decomposition of the H atom into its constituents: As will be seen, consistency with the NRQM result requires that Γ itself is singular when all the four momenta go on the mass shell.

In Sec. II below, I consider a simple nonrelativistic scenario which shows how the singularity structure of $g_{12}^{\rm Born}$ would be altered if the core electron were bound by a short-range force: There are then only *simple* poles. However, these are accompanied by branch points and in the limit of long-range binding, the singularities coalesce to form the higher-order poles.

A similar study shows that both the single and the double pole in the direct Born amplitude, considered as a function of the squared three-momentum transfer with the energy fixed, are also consequences of the long-range binding.

In Sec. III, the problem is examined from the viewpoint of Feynman diagrams and field theory, within the framework of an extemely simple model: The H atom is treated as if it were an elementary particle, described by a spin-zero field $\phi_{\rm H}$, coupled to electron and proton fieds ϕ_e and ϕ_p by a trilinear Lagrangian density $L_I = -G_0(\phi_e\phi_p)^\dagger\phi_{\rm H} + {\rm H.c.}$ The existence of a singularity at $k^2 \approx -\kappa^2$ of what appears to be the QFT counterpart of $g_{12}^{\rm Born}$ is then immediately manifest from a tree diagram, without the need to carry out any integrations.

In Sec. IV, I show that the model used in Sec. III is too simple to tell the full story: The nature of the singularity does not agree with that of the (Coulombic) NR theory-the tree graph has only a simple pole. Moreover, the counterpart of the direct amplitude has no pole at all in the square of the three-momentum transfer-there is a singularity at the appropriate point, but it is a branch point, rather than a pole: There is no free lunch. An analysis is given which indicates that the vertex function Γ must itself be singular when all particles are on the mass shell. Further aspects of the problem, from the view point of both NRQM and RQFT, are discussed in the final Sec. V.

II. NONRELATIVISTIC SCENARIO

The aim of this section is (i) to show that if the binding is by short-range forces, the singularity structure of both the exchange and direct Born amplitudes is the one naively expected from particle theory and (ii) to examine in detail how the higher-order poles arise when the forces become long range.

A. Exchange amplitude

We replace the hydrogen wave function ϕ by the so-called Hulthén wave-function χ, familiar from its use as an approximation to the deuteron wave function

$$\chi(\mathbf{r}_2) = N(\kappa,\lambda)[\exp(-\kappa r_2) - \exp(-\lambda r_2)]/r_2, \quad (2.1)$$

where $N(\kappa,\lambda)$ is a normalization constant, given by

$$N(\kappa,\lambda) = [\kappa\lambda(\kappa+\lambda)/2\pi(\kappa-\lambda)^2]^{1/2}. \quad (2.2)$$

For $\lambda > \kappa$, χ has the asymptotic form of a bound-state wave function appropriate for an interaction which decreases more rapidly than $1/r_2$, with associated binding energy $-\kappa^2/2m_e$. The advantage of this choice is that, as is readily verified, χ reduces to ϕ for $\lambda \to \kappa$, so that one can hope to follow the emergence of the higher-order poles. The Fourier transforms of ϕ and χ are

$$\begin{aligned}\tilde{\phi}(\mathbf{p}) &= (1/2\pi)^3 \int d\mathbf{r}_2 \exp(-i\mathbf{p}\cdot\mathbf{r}_2)\phi(\mathbf{r}_2) \\ &= (\kappa/\pi)^{5/2}(\mathbf{p}^2+\kappa^2)^{-2}, \end{aligned} \quad (2.3)$$

$$\begin{aligned}\tilde{\chi}(\mathbf{p}) &= (1/2\pi)^3 \int d\mathbf{r}_2 \exp(-i\mathbf{p}\cdot\mathbf{r}_2)\chi(\mathbf{r}_2) \\ &= [N(\kappa,\lambda)/2\pi^2][(\mathbf{p}^2+\kappa^2)^{-1} - (\mathbf{p}^2+\lambda^2)^{-1}]. \end{aligned} \quad (2.4)$$

Note that while $\tilde{\chi}(\mathbf{p})$ has only simple poles at $\mathbf{p}^2 = -\kappa^2$ and $\mathbf{p}^2 = -\lambda^2$, $\tilde{\phi}(\mathbf{p})$ has a double pole. It is the latter which is ultimately responsible for the double and triple poles in $g_{12}^{\rm Born}(k^2)$.

On using $\chi(\mathbf{r}_2)$ instead of $\phi(\mathbf{r}_2)$ in Eq. (1.1), writing

$$1/r_{12} = \int d\mathbf{q}(1/2\pi^2\mathbf{q}^2)\exp i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2), \quad (2.5)$$

setting $\mathbf{k}' = \mathbf{k}$, and integrating over the coordinates, one gets

$$g_{12}^{\rm Born}(k^2) = -(2/a\pi^2)\kappa\lambda(\kappa+\lambda)F(k;\kappa,\lambda)/(\kappa-\lambda)^2, \quad (2.6)$$

where

$$F(k;\kappa,\lambda) = I(k;\kappa,\kappa) + I(k;\lambda,\lambda) - 2I(k;\kappa,\lambda) \quad (2.7)$$

with

$$I(k;\kappa,\lambda)=\int d\mathbf{q}(1/\mathbf{q}^2)[(\mathbf{q}+\mathbf{k})^2+\kappa^2]^{-1}[(\mathbf{q}+\mathbf{k})^2+\lambda^2]^{-1}. \tag{2.8}$$

After combining the denominators in Eq. (2.8) with a Feynman parameter α, one can do the angular integration and a contour integration over q then yields

$$I(k;\kappa,\lambda)=\pi^2\int_0^1 d\alpha A^{-1}(k^2+A^2)^{-1}, \tag{2.9}$$

where $A^2=\alpha\kappa^2+(1-\alpha)\lambda^2$. Since $2AdA=(\kappa^2-\lambda^2)d\alpha$, the integration in Eq. (2.9) is elementary, with the result that

$$I(k;\kappa,\lambda)=[2\pi^2/k(\kappa^2-\lambda^2)]\times[\arctan(\kappa/k)-\arctan(\lambda/k)]. \tag{2.10}$$

For $\lambda\rightarrow\kappa$, $A\rightarrow\kappa$ and Eq. (2.9) gives

$$I(k;\kappa,\kappa)=\pi^2/\kappa(k^2+\kappa^2),$$
$$I(k;\lambda,\lambda)=\pi^2/\lambda(k^2+\lambda^2). \tag{2.11}$$

On inspection of Eqs. (2.6), (2.10), and (2.11) one sees that, regarded as a function of k in a complex k plane, $F(k;\kappa,\lambda)$ has both a simple pole and a logarithmic branch point at $k=\pm i\kappa$ as well as at $k=\pm i\lambda$. In the complex k^2 plane, these correspond to simple poles and branch points at $k^2=-\kappa^2$ and at $k^2=-\lambda^2$ for $g_{12}^{\mathrm{Born}}(k^2)$.

The triple and double poles of atomic theory can now be seen to arise from the coalescence of these singularities in the limit $\lambda\rightarrow\kappa$, as follows. On expanding $F(k;\ \kappa,\ \lambda)$ in powers of $\lambda-\kappa$ about the point κ, viz.

$$F=F^{(0)}+F^{(1)}(\lambda-\kappa)+F^{(2)}(\lambda-\kappa)^2/2!+\cdots, \tag{2.12}$$

one finds that the first two terms in Eq. (2.12) vanish, $F^{(0)}=F^{(1)}=0$, but that

$$F^{(2)}=\pi^2(3k^4+10k^2\kappa^2+15\kappa^4)/3\kappa^3(k^2+\kappa^2)^3. \tag{2.13}$$

This may be rewritten in the form

$$F^{(2)}=\pi^2\kappa^{-5}[(k^2/\kappa^2+1)^{-1}+(4/3)(k^2/\kappa^2+1)^{-2}+(8/3)(k^2/\kappa^2+1)^{-3}]. \tag{2.14}$$

On using Eq. (2.12) in Eq. (2.6), the $(\kappa-\lambda)^2$ factors are seen to cancel and one gets, in the limit $\lambda\rightarrow\kappa$, the form (1.3) for g_{12}^{Born} with

$$c_1=-2,\quad c_2=-8/3,\quad c_3=-16/3, \tag{2.15}$$

in agreement with the result of direct integration of Eq. (1.1). It should be noted that the value of the coefficient c_3 differs from that usually given in the literature. This is because the amplitude defined by Eq. (1.1) includes only the interaction of the incoming electron with the core electron and not also that with the proton, as emphasized by the subscript "12" on g. As mentioned, this point will be further discussed in Sec. V. In the Appendix, I show that, as one would expect, the absence of higher-order poles for short-range binding is quite general.

B. The direct amplitude

It will be useful to also consider in this interpolating model the direct amplitude f in the Born approximation, but this time as a function of the squared three-momentum transfer

$$\mathbf{Q}^2=(\mathbf{k}-\mathbf{k}')^2. \tag{2.16}$$

For the case of hydrogen, we have [1]

$$f^{\mathrm{Born}}(\mathbf{k},\mathbf{k}')=-(m_e/2\pi\hbar^2)\langle\mathbf{k}',\phi|-e^2/r_1+e^2/r_{12}|\mathbf{k},\phi\rangle=\langle\mathbf{k}'|V_\phi(r_1)|\mathbf{k}\rangle \tag{2.17}$$

with

$$V_\phi(r_1)=\langle\phi|-e^2/r_1+e^2/r_{12}|\phi\rangle=-e^2(1/r_1+1/a)\exp(-2\kappa r_1). \tag{2.18}$$

While the contribution from the first (Yukawa-like) term in Eq. (2.18) produces a simple pole, the second (pure exponential) term produces a double pole, both at $\mathbf{Q}^2=-4\kappa^2$

$$f^{\mathrm{Born}}(\mathbf{k}',\mathbf{k})=(2/a)[(\mathbf{Q}^2+\beta^2)^{-1}+\beta^2(\mathbf{Q}^2+\beta^2)^{-2}]\quad(\beta=2\kappa). \tag{2.19}$$

While a double pole is again unexpected from the viewpoint of field theory, in this case, even the single pole is a consequence of the long-range binding. To see this, note that on replacing ϕ by χ in Eq. (2.17) one gets

$$f^{\mathrm{Born}}(\mathbf{k}',\mathbf{k})=(m_e/2\pi(\hbar)^2)\langle\mathbf{k}'|V_\chi(r_1)|\mathbf{k}\rangle, \tag{2.20}$$

where

$$V_\chi(r_1)=\langle\chi|-e^2/r_1+e^2/r_{12}|\chi\rangle. \tag{2.21}$$

$V_\chi(r_1)$ is not an elementary function, but its form is not needed to evaluate f^{Born}. Using the representation (2.5), one finds

$$f^{\mathrm{Born}}(\mathbf{k}',\mathbf{k})=(2/a)F_\chi(\mathbf{Q}^2)/\mathbf{Q}^2, \tag{2.22}$$

where $F_\chi(\mathbf{Q}^2)$ is the charge form factor

$$F_\chi(\mathbf{Q}^2)=1-\int d\mathbf{r}_2\exp(-i\mathbf{Q}\cdot\mathbf{r}_2)\chi^2(\mathbf{r}_2). \tag{2.23}$$

Integration yields

$$F_\chi(\mathbf{Q}^2)=1-4\pi(N^2(\kappa,\lambda)/Q)[\arctan(Q/2\kappa)+\arctan(Q/2\lambda)-2\arctan(Q/(\kappa+\lambda)], \tag{2.24}$$

which has no poles but does have logarithmic branch points at $\mathbf{Q}^2 = -(2\kappa)^2$, $-(2\lambda)^2$, and $-(\kappa+\lambda)^2$. One readily verifies that in the limit $\lambda \to \kappa$, these branch points coalesce and that the single and double poles are regained.

Although the formula (2.19) for the direct Born amplitude is presumably much more familiar than that for the forward exchange amplitude (1.3), the fact that it displays poles in the squared momentum transfer does not seem to have drawn any attention in the literature.

C. Limit $\lambda \to \infty$

It is interesting to consider what happens in the limit $\lambda \to \infty$. This corresponds to extreme short-range binding, with

$$\chi(\mathbf{r}_2) \to \chi_0(\mathbf{r}_2) = N_0 \exp(-\kappa r_2)/r_2,$$
$$N_0 = N(\kappa,\infty) = (\kappa/2\pi)^{1/2}, \tag{2.25}$$

the wave function in the zero-range-force approximation. In this limit the second and third terms in Eq. (2.7) vanish, so that

$$F(k;\kappa,\lambda) \to I(k;\kappa,\kappa) = \pi^2/\kappa(k^2+\kappa^2). \tag{2.26}$$

It follows from Eq. (2.6) that

$$g_{12}^{\mathrm{Born}} \to -(2/a\pi^2)\kappa I(k;\kappa,\kappa) = -2a(k^2/\kappa^2+1), \tag{2.27}$$

which coincides with the first term in Eq. (1.2). This highlights the fact that it is precisely the second- and third-order poles which are related to the long-range Coulomb binding. The first-order pole is present (with the correct residue) even in the extreme short-range limit.

With regard to the direct Born amplitude in this limit, from Eqs. (2.24) and (2.22), one gets

$$f^{\mathrm{Born}} \to f_0 = (2/a)[1-(2\kappa/Q)\arctan(Q/2\kappa)]/Q^2. \tag{2.28}$$

Like the Coulomb result (2.19), f_0 is singular only at $Q^2 = -4\kappa^2$. However, the singularity is a branch point rather than the sum of first- and second-order poles.

III. SIMPLE FIELD-THEORY MODEL

In RQFT, the scattering of two particles is described by a Lorentz-invariant amplitude, the Feynman amplitude M. Let k, k' and K, K' denote the initial and final four momenta of the electron and hydrogen atom, respectively. The total four-momentum P, the four momentum transfer Q, and the "exchange four-momentum transfer" R are defined by

$$P = k+K, \quad Q = k-k', \quad R = k-K'. \tag{3.1}$$

The squares of these four vectors define the so-called Mandelstam variables,

$$s = P^2, \quad t = Q^2, \quad u = R^2, \tag{3.2}$$

satisfying the following relation:

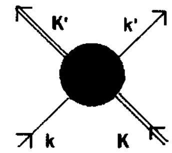

FIG. 1. Symbolic Feynman graph for the amplitude $M(s,t)$ describing $e^- - \mathrm{H}$ scattering. The solid lines represent the electron and the double lines the H atom.

$$s+t+u = 2m_e^2 + 2m_{\mathrm{H}}^2. \tag{3.3}$$

With spin ignored, as in the usual NRQM analysis, the Feynman amplitude for the process

$$e^- + \mathrm{H} \to e^- + \mathrm{H} \tag{3.4}$$

may be regarded as a function of s and t only,

$$M = M(s,t), \tag{3.5}$$

and represented by the symbolic Feynman diagram shown in Fig. 1. In this context, the analogs of the exchange and direct Born amplitudes would appear to be represented by the symbolic Feynman diagrams shown in Figs. 2 and 3, respectively. These involve the vertex function Γ for the virtual process $\mathrm{H} \leftrightarrow e^- + p$ and the vertex function Λ for the virtual process $\mathrm{H} \leftrightarrow \gamma + \mathrm{H}$. A discussion of these functions is deferred to Sec. IV. Let us first consider the problem within the context of a very simple field theory model and see how far we can get.

A. Exchange Feynman amplitude

Imagine that the H atom, in its ground state, can be treated as if it were an elementary particle, described by a field described by a scalar field ϕ_{H}, and that this field is coupled to complex scalar "electron" and "proton" fields ϕ_e and ϕ_p by a Lagrangian density

$$L_I = -G_0(\phi_e \phi_p)^\dagger \phi_{\mathrm{H}} + \mathrm{H.c.} \tag{3.6}$$

This can be regarded as a mock-up for the virtual process $\mathrm{H} \leftrightarrow e^- + p$, with the function Γ replaced by the constant G_0. The existence of an energy singularity at $\mathbf{k}^2 \approx -\kappa^2$ can then be inferred immediately from the tree-type diagram shown in Fig. 4, without the need to carry out any integrations.

To verify this assertion, note that the Feynman amplitude corresponding to Fig. 4 is given by

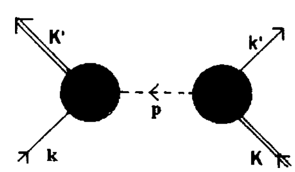

FIG. 2. Feynman-like graph associated with the simplest contribution to the exchange amplitude in $e^- - \mathrm{H}$ scattering. The dashed line represents the exchanged proton and the shaded circles denote the amplitudes for the virtual dissociation or formation of the H atom into or from its constituents.

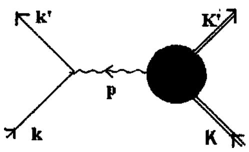

FIG. 3. Feynman-like graph associated with the simplest contribution to the direct amplitude in $e^- - \mathrm{H}$ scattering. The wavy line represents the exchanged photon and the shaded circle represents the electromagnetic vertex function of the H atom.

$$M_{\mathrm{ex}}^{(2)}(s,t)=G_0^2(u-m_p^2)^{-1}, \tag{3.7}$$

where m_p is the proton mass. On use of the relation (3.3), one sees that for $t=0$ (forward scattering) the pole of $M_{\mathrm{ex}}^{(2)}$ at $u=m_p^2$ corresponds to a pole $s=s_{\mathrm{ex}}$. with

$$s_{\mathrm{ex}}=2m_e^2+2m_{\mathrm{H}}^2-m_p^2, \tag{3.8}$$

Thus, the contribution of Fig. 4 to the forward exchange amplitude is

$$M_{\mathrm{ex}}^{(2)}(s,0)=G_0^2(s-s_{\mathrm{ex}})^{-1}. \tag{3.9}$$

To see what this corresponds to in terms of $\mathbf{k}^2$, the square of the three momentum of the electron in the center-of-mass system, note that in this system

$$k=(E_e,\mathbf{k}),\quad k'=(E_e,\mathbf{k}'),\quad K=(E_{\mathrm{H}},-\mathbf{k}),$$
$$K'=(E_{\mathrm{H}},-\mathbf{k}'), \tag{3.10}$$

where $E_e=(m_e^2+\mathbf{k}^2)^{1/2}$, $E_{\mathrm{H}}=(m_{\mathrm{H}}^2+\mathbf{k}^2)^{1/2}$. Then $s=(E_e+E_{\mathrm{H}})^2$ and a little algebra yields

$$\mathbf{k}^2=[s-(m_e+m_{\mathrm{H}})^2][s-(m_e-m_{\mathrm{H}})^2]/4s. \tag{3.11}$$

On using Eq. (3.8) in Eq. (3.11), one finds that the corresponding value of $\mathbf{k}^2$ is given by

$$\mathbf{k}_{\mathrm{ex}}^2=[(m_e-m_{\mathrm{H}})^2-m_p^2][(m_e+m_{\mathrm{H}})^2-m_p^2]/4s_{\mathrm{ex}}. \tag{3.12}$$

In terms of the physical binding energy ϵ', defined by

$$\epsilon'=m_e+m_p-m_{\mathrm{H}} \tag{3.13}$$

Eq. (3.12) takes the form

$$\mathbf{k}_{\mathrm{ex}}^2=(\epsilon'-2m_p)\epsilon'(2m_e-\epsilon')(2m_p+2m_e-\epsilon')/4s_{\mathrm{ex}}. \tag{3.14}$$

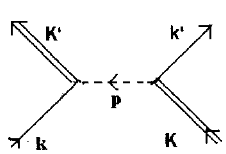

FIG. 4. Feynman graph associated with the simplest contribution to the exchange amplitude in $e^- - \mathrm{H}$ scattering. within the framework of the model defined by Eq. (3.6) of the text. The (*e, p*; H) vertex is associated with a factor $-iG_0$.

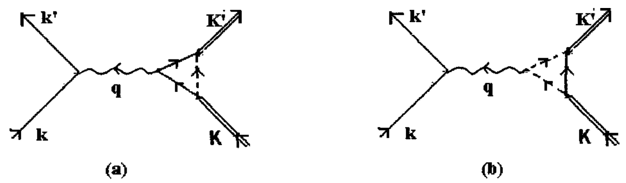

FIG. 5. (a), (b) Feynman graphs associated with the simplest contribution to the direct amplitude in $e^- - \mathrm{H}$ scattering, within the framework of the model defined by Eq. (3.6) of the text.

For the case at hand, $m_p \gg m_e \gg \epsilon'$, so that $s_{\mathrm{ex}} \to m_p^2$ and

$$\mathbf{k}_{\mathrm{ex}}^2 \to -2m_e\epsilon'. \tag{3.15}$$

On approximating ϵ' by the nonrelativistic value $\epsilon=\kappa^2/2m_e$, we see that in the limit of infinite proton mass and weak binding, we indeed recover a pole singularity at $-\kappa^2$. If one includes the leading recoil correction in Eq. (3.14) and to ϵ' the singularity is shifted to $-\kappa^2(1-2m_e/m_p)$. However, there is no sign of the higher-order poles.

B. Direct Feynman amplitude

The field theory analog of the direct Born term in NRQM is the amplitude for one-photon exchange, symbolized by Fig. 3. Application of the Feynman rules for emission of a photon by a spin-zero charged particle gives

$$-iM_{\mathrm{dir};1\gamma}(s,t)=-ie(k+k')^{\mu}(-ig_{\mu\nu}/q^2)(-i\Lambda^{\nu}), \tag{3.16}$$

where $q=k'-k$ and Λ^{ν} is the vertex function for emission of a virtual photon by the H atom. The general form of Λ^{ν} is

$$\Lambda^{\nu}=(K+K')^{\nu}F_+(t)+(K-K')^{\nu}F_-(t), \tag{3.17}$$

where the F's are charge form factors. Since $(k+k')\cdot(K-K')=(k+k')\cdot(-k+k')=0$ on the electron mass shell, we get

$$M_{\mathrm{dir};1\gamma}(s,t)=-e^2(k+k')\cdot(K+K')F_+(t)/t$$
$$=-e^2(s-u)F_+(t)/t. \tag{3.18}$$

The neutrality of the H atom requires that $F_+(0)=0$ so there is no pole at $t=0$, in agreement with Eqs. (2.22) and (2.23). The singularities of $M_{\mathrm{dir};1\gamma}$ are therefore determined by those of $F_+(t)$. In our model these are determined, to the lowest order in G_0, by the graphs shown in Figs. 5(a) and 5(b). The integrals associated with such triangle graphs are analytic functions in a complex t plane, with nearest branch points at $t_a>0$ and $t_b>0$, respectively. These would normally have the values associated with the threshold for pair production, $t_a=4m_e^2$ and $t_b=4m_b^2$, but because the H atom is weakly bound these thresholds are anomalous [6] and one finds that, e.g., $t_a \approx 4\kappa^2$, in agreement with Eq. (2.24). But, again there are no poles for $t>0$, i.e., for negative values of the squared three-momentum transfer.

IV. DEEPER ANALYSIS

While the simple model defined by Eq. (3.6) correctly yields the location of the singularity at $k^2=-\kappa^2$ of the exchange amplitude and that at $t=4\kappa^2$ of the direct amplitude, it does not yield the requisite analytic structure in the NR limit. The exchange amplitude has only a first-order pole and the direct amplitude has no pole at all. As usual in such cases, one suspects that the model is just too simple and that something has been neglected. It is however good enough to give the structure found in NRQM when the binding is short range. This suggests that we reexamine the amplitudes associated with Figs. 2 and 3 within the general context of RQFT.

By way of preparation, note that the amplitude Γ for the virtual decomposition of a spin-zero particle "3" into spin-zero particles "1" and "2," with four-momenta p_i $(i=1,2,3)$ constrained by $p_3=p_1+p_2$, may be written in the form

$$\Gamma=\Gamma(p_1,p_2). \tag{4.1}$$

Since Γ is a Lorentz scalar, it can be regarded as a function of the invariants p_1^2, p_2^2, and $p_1\cdot p_2$ or, equivalently, p_1^2, p_2^2, and $p_3^2=p_1^2+p_2^2+2p_1\cdot p_2$

$$\Gamma=\Gamma(p_1^2,p_2^2;p_3^2). \tag{4.2}$$

For the case at hand, identify particles 1, 2, and 3 with the electron, proton, and the H atom, respectively. Then the amplitude M' associated with Fig. 2 is

$$M_{\mathrm{ex}}'^{(2)}(s,t)=\Gamma(k^2,p_2^2;K'^2)(p_2^2-m_p^2)^{-1}\Gamma(k'^2,p_2^2;K^2). \tag{4.3}$$

The superscript "2" now indicates that M' is second order in Γ. The electron and the H atom are on the mass shell, $k^2=k'^2=m_e^2$ and $K^2=K'^2=m_{\mathrm{H}}^2$, while $p_2^2=(K-k')^2=u$ as in Eq. (3.2). On defining $\Gamma(p_2^2)$ for arbitrary p_2 by

$$\Gamma(p_2^2)=\Gamma(m_e^2,p_2^2;M_{\mathrm{H}}^2), \tag{4.4}$$

we have

$$M_{\mathrm{ex}}'^{(2)}(s,t)=\Gamma^2(u)(u-m_p^2)^{-1}, \tag{4.5}$$

where now

$$\Gamma(u)=\Gamma(m_e^2,u;M_{\mathrm{H}}^2). \tag{4.6}$$

The discussion in the preceding subsection would need no elaboration if the H atom were either an "ordinary" elementary particle, or a composite particle bound by short-range forces such as the deuteron. In either case, $\Gamma(u)$ will have the form

$$\Gamma(u)=\Gamma_0+\cdots, \tag{4.7}$$

where the dots denote terms which vanish when all the particles are on the mass shell and

$$\Gamma_0=\Gamma(m_e^2,m_p^2,M_{\mathrm{H}}^2). \tag{4.8}$$

Thus, near $u=m_p^2$

$$M_{\mathrm{ex}}'^{(2)}(s,t)=\Gamma_0^2(u-m_p^2)^{-1}+\cdots \tag{4.9}$$

and there is only a simple pole.

$M_{\mathrm{ex}}'^{(2)}(s,t)$ will have a singularity more complicated than a simple pole if and only if $\Gamma(u)$ is not analytic at $u=m_p^2$. In particular, if $\Gamma(u)$ itself has a simple pole at $u=m_p^2$, i.e., has the form

$$\Gamma(u)=a(u-m_p^2)^{-1}+b+c(u-m_p^2)+\cdots \tag{4.10}$$

in the neighborhood of m_p^2, then

$$M_{\mathrm{ex}}'^{(2)}(s,t)=a^2(u-m_p^2)^{-3}+2ab(u-m_p^2)^{-2}+(2ac+b^2)(u-m_p^2)^{-1}+\cdots, \tag{4.11}$$

which has precisely the singularity structure obtained in the nonrelativistic (Coulomb) calculation. Thus, it seems that consistency with the result of NRQM requires, at a minimum, that the $(e,p;\mathrm{H})$ vertex function $\Gamma(m_e^2,p_2^2;m_{\mathrm{H}}^2)$ has a pole at $p_2^2=m_p^2$. As in the nonrelativistic scenario, the existence of this pole must arise from the long-range character of the electron-proton interaction. However, there is still a problem with this relativistic scenario, discussed in the next section.

V. DISCUSSION

A. Comments on NR theory

The quantity g_{12}^{Born} defined by Eq. (1.1), considered in this paper as the Born approximation to the exchange amplitude, differs from that usually studied in the literature on electron-hydrogen scattering, which includes the interaction of the incoming electron with the core proton

$$g_1^{\mathrm{Born}}(\mathbf{k}',\mathbf{k})=-(m_e/2\pi\hbar^2)\langle\phi,\mathbf{k}'|-e^2/r_1|\mathbf{k},\phi\rangle. \tag{5.1}$$

The sum of Eqs. (5.1) and (1.1) is often referred to as the "Born-Oppenheimer approximation," a sobriquet apparently introduced by Mott and Massey [1]

$$g^{\text{Born-Opp}}=g_1^{\mathrm{Born}}+g_{12}^{\mathrm{Born}}. \tag{5.2}$$

A better name might be the "Oppenheimer-Born approximation." It appears first in a 1928 paper of Oppenheimer [7] and not in the famous paper of Born to which he makes reference. This would also avoid confusion with the universally known "Born-Oppenheimer approximation" for molecules. Evaluation of Eq. (5.1) yields

$$g_1^{\mathrm{Born}}(k^2)=ac_3'(k^2/\kappa^2+1)^{-3},\quad c_3'=16 \tag{5.3}$$

and the addition of Eqs. (5.3) to (1.3) changes the coefficient of the triple pole to $c_3+c_3'=-16/3+16=32/3$, in agreement with what is stated in the literature for the sum (5.2) [4].

Although the core term is not of direct interest for the purpose of this paper, it should be noted that this term was long a source of controversy, associated with the so-called "post-prior discrepancy" [1]. However, it was eventually shown by Day *et al.* [8] (see also Kang and Sucher [9]) that this discrepancy is "fictitious:" In an exact treatment, the rearrangement (or exchange) amplitude vanishes if the interaction between the incident and the bound particle is set equal to zero. This property, which makes good physical sense, is violated by the Oppenheimer-Born approximation. I have therefore omitted the core term in my analysis.

In any case, according to Amusia and Kuchiev [4], inclusion of some higher-order exchange effects changes the values of all the c_i. In the context of dispersion theory, precise knowledge of these coefficients would allow a more physically meaningful assessment of the importance of the discontinuities across the left-hand branch cuts.

Incidentally, a short calculation shows that in NRQM, the inclusion of recoil changes the position of the poles in k^2 from $-\kappa^2$ to $-\kappa^2(1+\eta)$ where $\eta = m_e/(m_e+m_p)$. Although such corrections are negligible for the case at hand, they would be significant for the analogous case of the low-energy scattering of a negative muon from a (μ^-,p) atom.

A by-product of Sec. II is the fact that only the second- and third-order poles are a consequence of the long-range binding; the first-order pole is there regardless of the nature of the binding. There has been some speculation in the literature linking the existence of the higher-order poles to the fact that in the static exchange approximation there are, in some cases, unexpected solutions to the effective one particle Schrödinger equation [3]. From the viewpoint of the present paper such an association is misleading: In the absence of binding by Coulomb forces the poles in the exchange amplitude are first order. It should be noted that in the analysis of Sec. II, the interaction of the incoming electron with the core proton plays no role; if one wishes, one may imagine that this Coulomb interaction may also be replaced by the same short-range force which leads to the wave-function χ for the bound electron, so as to be conceptually consistent with the identity of the incoming and bound particles.

B. Field-theoretic aspects

Independent of the nature of the singularities, there is another problem with the simple field theory model of Sec. III. This is the fact that the NR exchange amplitude, as defined by Eq. (1.1), obviously vanishes if there is no direct interaction between the incoming and bound electrons, i.e., if $e^2/r_{12} \to 0$. However, the graph of Fig. 2 and *a fortiori* that of Fig. 3, does not involve any direct interaction between these particles. It therefore seems likely that in a genuine field-theoretic calculation the contribution of this graph vanishes in the infinite mass limit and that the "true" exchange amplitude, that is the one which agrees with NRQM in the NR limit, comes from a graph in which Fig. 2 is modified by the insertion of the exchange of a single photon between the electron line, as shown in Fig. 6. Although such a graph normally has only branch-point singularities, nothing is normal here. The expected pole in the vertex function Γ may convert a branch point into a pole in the overall amplitude, by acting like a derivative with respect to an internal mass. Similarly, agreement with the NR theory of the direct amplitude is likely to be obtained if the full Γ is used in the calculation of the form factor Λ. In a further study, it would be interesting to test these conjectures. From a methodological point of view, one might gain further insight into the nature of the the left-hand singularities, beyond the Born approximation.

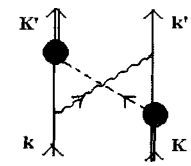

FIG. 6. Feynman-like graph associated with a contribution to the exchange amplitude involving both photon and proton exchange.

Finally, it is worthwhile noting that the problem of elastic neutron-deuteron scattering is conceptually very similar to that of e^--H scattering. Instead of two electrons and a proton, with one electron bound to the proton, one has two neutrons and a proton, with one of the neutrons bound to the proton. The vertex function for the virtual process $d \to n + p$ is expected to be well defined when all the nucleons are on the mass shell and its value there is simply regarded as the $(n,p;d)$ coupling constant. Because of the long-range binding, it seems that the analogous object, an $(e,p;\mathrm{H})$ coupling constant, does not exist. In future work, it would be desirable to establish, by direct calculation, that in a fully relativistic theory the $(e^-,p;\mathrm{H})$ vertex function with only the proton off the mass shell, $\Gamma(m_e^2,p_2^2;m_\mathrm{H}^2)$, has the structure exhibited in Eq. (4.10).

In conclusion, it seems safe to say that in the ancient problem of electron-hydrogen scattering there are still lessons to be learned, for both atomic and particle physics.

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APPENDIX

In the text it was asserted that if the binding potential is short range, i.e., decreases more rapidly that $1/r$ for large r, then the singularities of the Born terms are those expected from field theory. However, this was only illustrated by the simple example of the Hulthén wave function, which allowed all the integrations to be carried out explicitly. It is straightforward to see that the result is quite general.

Consider the large class of wave functions which admit a spectral representation of the form

$$\phi(r) = \int_0^\infty d\mu \rho(\mu) \exp(-\mu r). \tag{A1}$$

For $\rho(\mu)=N\theta(\mu-\kappa)\theta(\lambda-\mu)$, this reduces to Eq. (2.1) of the text. In this special case, the correction to the leading term at large r is itself exponential in form. Normally, one would expect inverse power corrections to $N\exp(-\mu r)/r$. Indeed, with $\rho(\mu)=\theta(\mu-\kappa)\sigma(\mu)$ and $\sigma(\mu)$ differentiable at $\mu=\kappa$, we get, on repeated integration by parts,

$$\phi(r)=\exp(-\mu r)[\sigma(\kappa)/r+\sigma'(\kappa)/r^2+\sigma''(\kappa)/r^3+\cdots], \tag{A2}$$

corrections of the usual form. Assume that $\sigma(\mu)$ is bounded for large μ. Then the Fourier transform of Eq. (A1) is given by

$$\phi(p)=\text{const}\int_\kappa^\infty d\mu\,\sigma(\mu)/(p^2+\mu^2)^2. \tag{A3}$$

This is manifestly an analytic function of p^2, singular only at $p^2=-\kappa^2$. Integration by parts yields

$$\phi(p)=\phi_1(p)+\phi_2(p), \tag{A4}$$

where, with $g(\mu)=\sigma(\mu)/2\mu$,

$$\phi_1(p)\propto g(\kappa)/(p^2+\kappa^2), \quad \phi_2(p)\propto\int_\kappa^\infty d\mu\,g'(\mu)/(p^2+\mu^2). \tag{A5}$$

$\phi_2(p)$ exhibits the pole associated with $\exp(-\mu r)/r$, while $\phi_2(p)$ is an analytic function of p^2, with a logarithmic branch point at $p^2=-\kappa^2$. On using the form (A4) instead of Eq. (2.4) in the calculation of the exchange Born amplitude, one sees that the ''1-1'' term will yield the simple pole term analogous to $I(k;\kappa,\kappa)$ in Eq. (2.11) while the ''2-2'' and the mixed terms will yield only branch-point singularities; no higher-order poles appear.

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