Multiple Pole in the Electron–Hydrogen-Atom Scattering Amplitude

M. Ya. Amusia and M. Yu. Kuchiev
Ioffe Physical-Technical Institute of the Academy of Sciences, Leningrad, U. S. S. R.
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It is demonstrated that the amplitude for electron–hydrogen-atom forward scattering has the third-order pole at the point $E=-13.6$ eV, E being the energy of the incident electron. The coefficients which characterize the pole are calculated exactly. The invalidity of the Born approximation is proved. The contribution of the pole singularity to the dispersion relation for the scattering amplitude is discussed.

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In this paper we consider the singularities of the forward electron-atom scattering amplitude in the complex plane of the energy E of the incoming electron. The interest in the analytical structure of the amplitude originates from the fact that all the singularities in the E plane contribute to the dispersion relation which was recently carefully checked by using modern experimental and theoretical data.[1-5]

Let us consider electron scattering by the simplest hydrogen atom. The amplitude for $e+\mathrm{H}$ forward scattering has a cut on the semiaxis $E\geq 0$ and a pole at the binding energy $E=E_-=-0.76$ eV of the negative ion H^-. Both of these singularities are similar to those for the case of potential scattering.

The behavior of the amplitude on the real energy axis for $E<E_-$ has been discussed in Refs. 6–8. It was demonstrated that the amplitude is regular up to the atomic binding energy $E=E_0=-13.6$ eV. At this point the amplitude is singular, the singularity being the result of the possible exchange between the atomic and incoming electrons. Singularities of this kind are well known in nuclear and elementary-particle physics. However, the structure of the singularity at the atomic binding energy is quite specific as a result of the long-range nature of the Coulomb potential.

To clarify it let us suppose for a moment that the mass of the photon has some small finite value λ. The Coulomb potential in this case has the form $(-e^2/r)\exp(-\mu r)$, where $\mu=c\lambda/\hbar$. Then the exchange diagram in Fig. 1(a) has an ordinary pole[9] at the binding energy of the atom $E=E_1=-\hbar^2\kappa^2/2m$, $E_0<E_1$. All of the rest of the exchange diagrams have rather complicated Landau singularities on the semiaxis $E\leq E_2=-\hbar^2(\kappa+\mu)^2/2m<E_0$.[6] When we proceed to the limit of zero photon mass, $\lambda\to 0$, the pole at $E=E_1$ and the right edge of the Landau singularities at $E=E_2$ move to the same point $E=E_0$; that is, the singularities concentrate at this point. Therefore the behavior of the $e+\mathrm{H}$ scattering amplitude at $E=E_0$ (and in the region $E\leq E_0$) is *a priori* unknown.

First, in Ref. 10 in the static exchange approximation and in Refs. 6 and 7 in the second Born approximation it was demonstrated that the non-Born part of the scattering amplitude is singular at the point $E=E_0$. The trouble, however, is that all of the exchange diagrams are singular at this point.[6] In this work we succeed in summing them precisely. It is convenient to start from the diagram presented in Fig. 1(b). The analytical expression for it is ($e=\hbar=m=1$)

$$g_1(k)=-(2\pi)^{-4}\int(4\pi/q^2)\varphi_{1s}{}^2(\vec{\mathrm{k}}-\vec{\mathrm{q}})d^3q\,. \tag{1}$$

In (1) $k=(2E)^{1/2}$ denotes the momentum of the incoming electron, $\vec{\mathrm{q}}$ is the transferred momentum, and $\varphi_{1s}(p)=8\pi^{1/2}(p^2+1)^{-2}$ is the Fourier component of the ground-state wave function for the hydrogen atom. We are interested in the amplitude behavior in the limit $k^2+1\to 0$. Let us scale the integration variable: $\vec{\mathrm{q}}-\vec{\mathrm{Q}}=(k^2+1)^{-1}\vec{\mathrm{q}}$. Then (1) transforms into the following expression:

$$g_1(k)=-16\pi^{-2}(k^2+1)^{-3}\int Q^{-2}[\,1-2\vec{\mathrm{k}}\cdot\vec{\mathrm{Q}}+(k^2+1)Q^2\,]^{-4}d^3Q=\tfrac{16}{3}(k^2+1)^{-3}+\text{higher-order terms}\,. \tag{2}$$

We can see that $g_1(k)$ has a third-order pole at $k^2+1=0$. In calculating the numerical coefficient $-\frac{16}{3}$ in (2) it is possible to neglect the term proportional to Q^2 compared with $\vec{\mathrm{k}}\cdot\vec{\mathrm{Q}}$ in the denominator of the integrand. It is significant that the same result may be obtained for an arbitrary diagram of the exchange amplitude. In our approach both electrons in the intermediate states are described by plane waves. Hence every energy denominator of an arbitrary diagram [for example Fig. 1(c)] is quadratic in the momenta $\vec{\mathrm{q}}_1,\ldots,\vec{\mathrm{q}}_n$ transferred during the Coulomb interaction. It is easy to find that in the vicinity of the

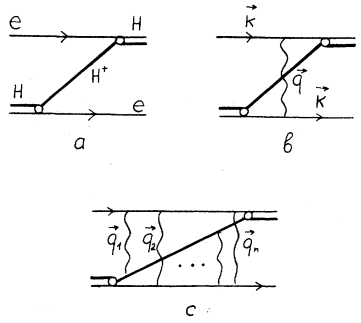

FIG. 1. Some Feynman diagrams describing the exchange amplitude of e + H scattering. The solid line represents the propagation of the free electron. The double line corresponds to the ground hydrogen-atom state. The wavy line describes the Coulomb interaction.

point $k^2+1=0$ every denominator becomes small for small transferred momenta $q_i \lesssim |k^2+1|$, $i=1,\ldots,n$. Consequently the region of small transferred momenta is very essential. In order to consider this region in detail it is convenient to make the scaling substitution $\vec{q}_i \to \vec{Q}_i = (k^2+1)^{-1}\vec{q}_i$. Using it we reduce the expression for every energy denominator E_j, $j=1,\ldots,n+1$, to the following one:

$$E_j = -\tfrac{1}{2}(k^2+1)[\,1 - 2\vec{k}\vec{P}_j + (k^2+1)A_j\,]. \qquad (3)$$

Here $\vec{P}_j$ is a linear combination of $\vec{Q}_1,\ldots,\vec{Q}_n$ and A_j is quadratic in the same variables. The representation (3) shows that about the point $k^2+1=0$ all the items quadratic in transferred momenta are negligible compared with the linear items. Consequently the well-known eikonal approximation[11] gives the exact asymptotic behavior of the exchange amplitude. This is a rather surprising result. Usually the eikonal approximation is applied when the energy of the incoming particle is sufficiently large.[12]

The expression (3) permits us to show that each exchange diagram has a third-order pole at $k^2+1=0$. In order to sum the diagrams it is convenient to pass to the time description of the process using the formula

$$E_j^{-1} = -i\int_0^\infty \exp(-it_j E_j)\,dt_j\,.$$

Since E_j (in the eikonal approximation) is linear in the transferred momenta $\vec{q}_1,\ldots,\vec{q}_n$, the time representation permits us to evaluate the integrals over all $\vec{q}_i$. Consequently one obtains an expression for a diagram where only the integrals over different intervals of time remain. Simple algebraic transformations permit the representation of the sum of all exchange diagrams in the nth order ($n \geq 2$) of the perturbation theory as

$$g_n(k) = 2i\int_0^\infty dt\int_0^t dt_2\int_0^{t_2} dt_1 \frac{1}{(n-2)!}\left[-i\int_{t_1}^{t_2}\left(\frac{1}{kt}-\frac{1}{k\tau}-\frac{1}{k(t-\tau)}\right)d\tau\right]^{n-2}$$
$$\times\left(\frac{1}{kt}-\frac{1}{k(t-t_1)}\right)\left(\frac{1}{kt}-\frac{1}{kt_2}\right)t_1(t-t_2)\exp[\,it(E_0-\tfrac{1}{2}k^2)\,] + \text{higher-order terms}\,. \qquad (4)$$

Summing $g_n(k)$ in (4), we find the expression for the exchange amplitude:

$$g(k) = g^{\text{eik}}(k) + \text{higher-order terms};$$

$$g^{\text{eik}}(k) = g_B(k) + 2i\int_0^\infty dt\int_0^t dt_2\int_0^{t_2} dt_1\left(\frac{1}{kt}-\frac{1}{k(t-t_1)}\right)\left(\frac{1}{kt}-\frac{1}{kt_2}\right)t_1(t-t_2)$$
$$\times\exp\left[it(E_0-\tfrac{1}{2}k^2) - i\int_{t_1}^{t_2}\left(\frac{1}{kt}-\frac{1}{k\tau}-\frac{1}{k(t-\tau)}\right)d\tau\right]. \qquad (5)$$

Here $g_B(k)$ is the contribution of the diagrams of Figs. 1(a) and 1(b) which coincides with the well-known Born-Oppenheimer amplitude. These diagrams are easily calculated either directly or in the eikonal approximation with, of course, the identical result. Representation (5) has a clear physical interpretation. The exchange process lasts the interval t. During this time both electrons are moving rectilinearly with the velocity $\vec{k}$. The exponent in (5) includes the usual eikonal expression, the classical action calculated for rectilinear trajectories. The first multiplier of the integrand is simply the incoming-electron–atom interaction potential. Analogously, the second multiplier describes the outgoing-electron–atom interaction. The multipliers t_1 and $t-t_2$ arise from the transformation of atomic wave functions into time representation.

After simple calculation we find from (5)

$$g(k) = (32/e)(k^2+1)^{-3} + \text{higher-order terms}. \qquad (6)$$

Here $e = 2.718\ldots$.

The eikonal approximation permits us to prove the existence of the multiple pole (6). To calculate the values of the coefficients for $(k^2+1)^{-2}$ and $(k^2+1)^{-1}$ terms in the amplitude it is necessary to expand the integrand for each diagram [see, for example, formula (2) corresponding to the diagram of Fig. 1(b)] in powers of k^2+1 with an accuracy to the second order. In this way we find corrections to the simple eikonal expression (5). This calculation is sufficiently complicated and therefore cannot be described in detail within the framework of this paper. The final expression for the pole term in the exchange amplitude is

$$g(k) = g_p(k) + \text{higher-order terms};$$

$$g_p(k) = \frac{32}{e}(k^2+1)^{-3} - \frac{16}{3e}(k^2+1)^{-2} + \frac{1}{e}\left(\frac{4\pi^2}{3} - \frac{167}{15}\right)(k^2+1)^{-1}. \tag{7}$$

Earlier[1] it was shown that the Born-Oppenheimer amplitude has a third-order pole,

$$g_B(k) = \tfrac{32}{3}(k^2+1)^{-3} - \tfrac{8}{3}(k^2+1)^{-2} - 2(k^2+1)^{-1}. \tag{8}$$

It was a general belief that such an unusual behavior is a peculiar feature of the Born approximation, which is equal to the sum of the graphs in Figs. 1(a) and 1(b). We have shown that the pole behavior is inherent to every exchange diagram. It should be noted that the difference between (7) and (8) is prominent. In particular the signs of the residues are opposite.

Let us consider now the contribution from the pole at $k^2+1=0$ to the dispersion relation for the forward $e+H$ scattering amplitude. The structure of the amplitude singularities in the complex energy plane discussed above leads to the following dispersion relation (DR):

$$\mathrm{Re}F(k) - f_B - \frac{1}{4\pi^2}\int_0^\infty \frac{(2E')^{1/2}\sigma_t(E')}{E' - k^2/2}\,dE' - \frac{d_-}{k^2/2 - E_-} = u(k). \tag{9}$$

Here $F(k) = f(k) - \frac{1}{2}g(k)$ is a linear combination of the direct and exchange amplitudes constructed so that the optical theorem for it is fulfilled. The third and fourth terms of the left-hand part of expression (9) are connected with the cut on the right semiaxis $E \geq 0$ and with the pole at the binding energy of the negative ion H^-. The function $u(k)$ in (9) includes the singularities in the amplitude which appear as a result of the possible exchange. If one assumes that the pole (7) is the only singularity of the latter type then the expression for $u(k)$ reduces to the following one:

$$u_p(k) = -\tfrac{1}{2}g_p(k). \tag{10}$$

The DR (9) was first considered for $e+H$ scattering by Gerjuoy and Krall.[1] They assumed that the function $u(k)$ in (9) is determined by the Born amplitude,

$$u_{GK}(k) = -\tfrac{1}{2}g_B(k). \tag{11}$$

The functions $u_p(k)$ and $u_{GK}(k)$ as well as the left-hand part of the DR (9) obtained by Heer, McDowell, and Wagenaar[5] are presented in Fig. 2. Note that the curves for $u_p(k)$ and the left-hand part of the DR are in qualitative agreement in the region $k^2 > 1$ where their signs are equal.

The quantitative difference between them for $k^2 < 1$ can be caused by two reasons. Firstly, the above consideration shows that besides the multiple pole other singularities of the exchange amplitude may exist on the semiaxis $E \leq E_0 = -0.5$. Secondly, the available data on the $e+H$ scattering cross section for intermediate energies are not quite satisfactory. It was pointed out[4] that the variation of the cross section affects sub-

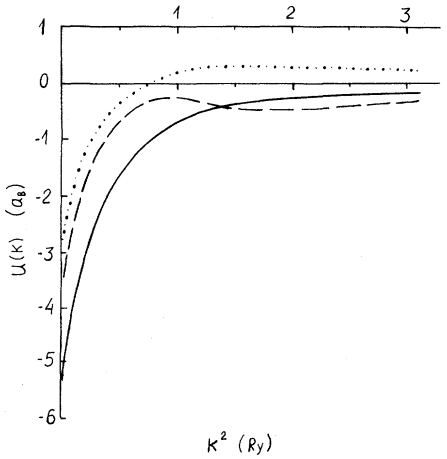

FIG. 2. The solid line represents the function $u_p(k)$, Eq. (10). The dashed line represents the left-hand part of the DR, Eq. (9), calculated in Ref. 5. The dotted line is the Born approximation $u_{GK}(k)$, Eq. (11).

stantially the left-hand side of the DR (9) for small energies.

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[12]Note that in our case the propagation of both electrons is described in the eikonal approximation. This is different from the Glauber approach where only one fast particle is described in the eikonal spirit.