ON THE PROTON EXCHANGE CONTRIBUTION TO ELECTRON-HYDROGEN ATOM ELASTIC SCATTERING

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ABSTRACT - It is shown that the exchange contribution to the electron-proton potential Born term in elastic electron-hydrogen atom scattering arises as the non relativistic limit from the exchange of a proton between the two participant electrons _ calculated from quantum electrodynamics including properly bound states (as solution of Bethe - _ Salpeter equation).

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I. INTRODUCTION

It is currently admitted that the interaction between charged particles in ordinary non relativistic quantum mechanics is obtained from the appropriate non relativistic limit of quantum electrodynamics. Expressions for the inter - action between charged particles and particles and anti - particles can be found, for instance, in the book by Lifshitz, Berestetsky and Pitaevsky [(1)].

If, beyond, we want to study the interaction of charged particles with more complex systems of charged particles such as atoms, we need to include in the frame - work of the theory a fortiori a suitable treatment of bound states. The problem for two body bound states in a relativistic quantum description has been solved formally more than a quarter of a century ago by Y.Nambu, E.E. Salpeter and H. Bethe and M.Gell-Mann and F. Low[(2)]. In fact, approximate solutions in quatum electrodynamics became available only last year[(3)].

A pure potential scattering description of the scattering of charged particles by atomic systems is not accurate since polarization effects are needed to be accoun-ted for. Nonetheless, it is an interesting problem to investigate for these physical systems how the potential theory description in terms of the Born series and the non-relativistic limit of the more elaborate (and fundamental) theory match.

The introduction of bound states as possible asymptotic states in a relativistic quantum scattering theory was first studied by Eden in a series of papers[4] unjustly not very often mentioned in the current literature on this subject. There, a modified interaction picture was introduced that summed up the effect of that part of the hamiltonian responsible for the bound states, and the perturbative series was built through the usual methods on the rest. An expression for the whole two body propagator allowing for the interaction of the constituents with external particles was introduced by Eden and Rickayzen[4]. Subsequently, Mandelstam [5] extended Eden results to general matrix elements of fields including bound states, and an axiomatic treatment was later formulated by R.Haag, K. Nishijima and W.Zimmermann in separate contributions[6].

The explicit calculation of the Born terms for electron-hydrogen atom elastic scattering was performed as an application by Eden and Rickayzen*[4]. In terms of Feynman graphs, they calculated the contributions appearing in Fig. 1. These, from a S-matrix point of view, describe a set of three crossed channel contributions coming respectively from the exchange of a Coulomb photon between the incident electron and the electron and the proton constituents of the hydrogen atom (Figs.1a and 1b), and a separate contribution from the exchange of both electrons (fig. 1c). In a potential theory description they correspond rigorously to the Coulomb interaction Born contribution, to which they tend when the non relativistic limit is taken.

There is, however, a fourth term in the Born

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*Unfortunately, this article is marred by a lot of misprints and by an unorthodox way of writing fermion propagators.

term, the incident electron-proton interaction including exchange. This is a somewhat controversial contribution, since some authors claim that it can be obtained from higher orders in perturbation theory[7].

There is also in field theory a conceivable contribution to this process, since one notices that the crossed positron-hydrogen atom elastic scattering channel admits the quantum numbers of the single proton. It would arise from the set of graphs like the ones depicted in Fig. 2, where a proton propagates alone "after" interacting with one electron and "before" interacting with the other. The corresponding sum of all these diagrams is represented in Fig. 3, and it is clearly another exchange contribution, the exchange of a proton between both electrons. A similar contribution has been known since a rather long time in neutron-deuteron elastic scattering[8]. A careless extrapolation of S-matrix usual arguments would propose that this contribution would be of order 1/M (M being the proton rest mass), and that it would contribute mainly backwards.

Instead, when we calculated it, as is shown in the next section, we found that in the non-relativistic limit it corresponds precisely to the fourth contribution in the potential scattering first Born term mentioned earlier, the electron-proton scattering with exchange. Moreover, it does not prefer the backward direction, and it is of the same order in potential theory as its corresponding radiative correction, Fig. 1c). The fact that the exchange of a massive particle in the crossed channel is somewhat related to a long range potential warns again naïve application of ideas born in a framework into another.

In the next section we shall proceed to the calculation of this contribution starting mainly from first principles. The same result comes from the application of Blankenbecler, Goldberger and Halpern methods[8]. The end section discusses the derivation of this result and possible applications, especially in rapport with the application in atomic scattering theory.

2. CALCULATIONS

This section spans in two parts. The first one is related to the kinematics, and the second with the calculation of the proton exchange term.

Let $p_e(p'_e)$ and $P(P')$ be the initial (final) momenta of the electron and the hydrogen atom, respectively. The usual well known three relativistic channels corresponding to this process and related by crossing symmetry are*:

i) s-channel, for the process $e^- + H \rightarrow e^- + H$, with a total four momentum $K = p_e + P$, $(= p'_e + P')$ and with $s = K^2$ as a scalar invariant related to the total energy in the center of momentum frame.

ii) t-channel, corresponding in this case to the process $e^- + e^+ \rightarrow \bar{H} + H$ when the four momentum transfer $\Delta = p_e - p'_e$ is time like, and with the scalar invariant

$$t = \Delta^2 \qquad (< 0 \text{ for the s-channel process})$$

iii) u-channel, corresponding here to the process $e^+ + H \rightarrow e^+ + H$ when the crossed four momentum transfer $Q = p'_e - P$ is

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*We take $\hbar = c = 1$

time-like, and with associated scalar invariant

$$u = Q^2 \quad (< 0 \text{ for the s-channel process})$$
$$= 2\, M_H^2 + 2m^2 - s - t$$

where M_H is the hydrogen atom rest mass in its ground state and m is the electron rest mass.

We stop for a moment to give a detailed calculation that enlights the meaning of the value $u = M^2$ in the non-relativistic limit. We shall work in the laboratory frame, but the final result is not modified when taking the limit $M \to \infty$ in this frame or in the center of momentum frame. We then have $\vec{P} = 0$, $E_H = M_H$ and

$$u = m^2 + M_H^2 - 2\, E'_e\, M_H \tag{1}$$

or

$$E'_e(u) = (m^2 + M_H^2 - u)/(2M_H) \tag{1'}$$

Taking $u = M^2$ and writing for the mass and binding energy of the hydrogen atom the definition

$$M_H = M + m - \varepsilon \tag{2}$$

we have:

$$E'_e(u{=}M^2) = \left[2Mm + m^2 - 2(M{+}m)\varepsilon + \varepsilon^2\right] (2M)^{-1} \left[1 + \frac{m-\varepsilon}{M}\right]^{-1} \tag{3}$$

Taking into account that $\varepsilon << m << M$

$$E'_e(u=M^2) = (m-\varepsilon) + \frac{1}{2}\frac{m}{M}(m-\varepsilon) - \frac{1}{2}\frac{(m-\varepsilon)^2}{M} +$$

$$+ \frac{1\varepsilon^2}{2M} + 0\left(\left(\frac{m}{M}\right)^2, \left(\frac{\varepsilon}{M}\right)^2\right) \qquad (4)$$

Since $E'^2_e = \vec{p}'^2_e + m^2$, we can develop both sides in the non-relativistic approximation and find

$$\vec{p}'^2_e\,(u=M^2) + 2\,m\,\varepsilon = 0 \qquad (5)$$

up to orders $\left(\frac{p'^2_e}{m^2}\right)^2$, $\frac{\varepsilon}{M}$, $\frac{m}{M}$, the last two being negligible when $M \to \infty$, as it is taken for the calculation of low energy scattering in the Born series. The above expression looks like the non relativistic condition for the existence of the bound state if $\vec{p}'^2_e$ were the square of the relative three-momentum of the hydrogen atom. In fact it appears as such in the calculation that follows.

We shall use the Coulomb gauge[(1)]

$$\nabla \cdot \vec{A} = 0$$

where the photon propagator in momentum space is

$$D_{ij}(k) = -4\pi(k^2)^{-1}(\delta_{ij} - k_i k_j |\vec{k}|^{-2})$$

$$i,j = 1,2,3 \qquad (6a)$$

$$D_{0i}(k) = 0 \qquad i=1,2,3 \tag{6b}$$

$$D_{00}(k) = -4 \, |\vec{k}|^{-2} \tag{6c}$$

and our conventions for Feynman rules are the ones contained in Ref.1) page 361.

We shall follow the guide-lines that can be found in K.Nishijima's book(9). They are quite similar to the procedures advanced by Eden and Rickayzen(4) and developed by Mandelstam(5). They lead to the same results as applying formally the method of Blankenbeler et al.(8) which was obtained for and applied to neutron-deuteron elastic scattering.

The content is to start from the three body to three body scattering amplitude, join two particles in a common two-body propagator in the initial and final state, and then calculate the residue of the amplitude at the pole of the two body propagators.

Use will be made of the one particle and two particle Feynman amplitudes

$$\mathcal{F}'_{a}(x) = < \Psi_0^{(-)}, \Psi_a^H(x) \; \Psi_a^{(+)} > \tag{7}$$

$$\mathcal{F}_{ab}(x_1,x_2) = \mathcal{F}(12;\ ab) =$$

$$= < \Psi_0^{(-)}, \; T\left[\Psi_a^H(x_1) \; \Psi_b^H(x_2)\right] \; \Psi_{ab}^{(+)} > \tag{8}$$

where Ψ_i is a zero, one or two particle state, + or - refer to incoming and outgoing states and $\Psi_i^H(x)$ is the Heisenberg field of particle i. The two particle Feynman amplitude satisfy a Bethe Salpeter equation

$$\mathcal{F}(12;ab) = \mathcal{F}_a(1)\,\mathcal{F}_b(2) + \int d3\; d4\; d5\; d6\; K_F^a(1,3)\; K_F^b(2,4)\,G(34;56)\,\mathcal{F}(56;ab) \qquad (9)$$

where $K_F^i(\ell,m)$ is the complete one particle propagator and G is the kernel. For a bound state, $\mathcal{F}(12;B)$ satisfies the homogeneous Bethe Salpeter obtained from (9) that may also be written as

$$\int d\,1'\; d\,2'\; K_F^{a^{-1}}(1,1')\; K_F^{b^{-1}}(2,2')\; \mathcal{F}(1'2';B) = \int d5\;\; d6\;\; G(12;56)\;\mathcal{F}(56;B) \qquad (10)$$

A ladder solution is obtained when solving (9) or (10) with a kernel of the form:

$$G(12;56) = \delta\,(1,5)\,\delta\,(2,6)\quad G'(1,2) \qquad (11)$$

where G'(i,j) is the propagator of a particle or of the proton (in QED) and $\delta\,(i,j)$ is a Kronecker and/or Dirac delta. A formal solution of Eqs. (9) or (10) is of the form:

$$\mathcal{F}(12;ab) = \mathcal{F}_a(1)\,\mathcal{F}_b(2) + \int d3\;\; d4\;\; d5\;\; d6\;\; K_{ab}(12;34)\,G(34;56)\,\mathcal{F}_a'(5)\,\mathcal{F}_b(6) \qquad (12)$$

where

$$K_{ab}(12;34) = < \Psi_0^{(-)}, T \left| \Psi_a^H(x_1) \quad \Psi_b^H(x_2) \quad \Psi_a^H(x_3) \quad \Psi_b^H(x_4) \right| \Psi_0^{(+)} > \tag{13}$$

is the two body propagator for particles a and b, that also satisfies a Bethe Salpeter equation.

Let us then start from the three-particle to three particle transition amplitude

$$< e_2 \; p_2 \; e'_2 \; |S - 1| \; e_1 \; p_1 \; e'_1 >= \int d^4y_e \; d^4y_p \; d^4y_{e'} \; d^4x_e \; d^4x_p d^4x_{e'}$$

$$\tilde{\mathcal{F}}_{e_2}(y_e)\tilde{\mathcal{F}}_{p_2}(y_p)\tilde{\mathcal{F}}_{e'_2}(y_{e'})\, \sigma(y_e{:}y_p{:}y_{e'};x_e{:}x_p{:}x_{e'})\, \mathcal{F}_{e_1}(x_e)\mathcal{F}_{p_1}(x_p)\mathcal{F}_{e'_1}(x_{e'}) \tag{14}$$

Let us now consider that e_2,p_2 and e_1,p_1 are propagating together. This amounts to consider the following relationship between the nuclei of the amplitudes:

$$\sigma(1{:}2{:}\ldots) = \sigma(12{:}\ldots) + \int d3 \; d4 \; d5 \; d6 \; G(12,34) \; K(34;56)\sigma(56{:}\ldots) \tag{15}$$

and we do not consider the inhomogeneous term, since it does not contribute when considering the propagation of a bound state. Here the notation makes evident that we have gathered the coordinates of two particles. Writing the resulting expression in a condensed way

$$<(e_2p_2)e'_2 \; |S-1| \, (e_1p_1)_H e'_1> =$$

$$= \int \ldots \tilde{\mathcal{F}}_{e_2} \tilde{\mathcal{F}}_{p_2} \tilde{\mathcal{F}}_{e'_2} \; \sigma(e_2p_2;\ldots) K(\ldots;\ldots) \sigma(ep:e';ep:e')$$

$$K(\ldots;\ldots) \; G(\ldots;e_1p_1) \mathcal{F}_{e_1} \mathcal{F}_{p_1} \mathcal{F}_{e'_1} \qquad (16)$$

Using the formal solution of the two particle Feynman amplitude we arrive at

$$<(e_2p_2)_H \; e'_2 \; |S-1| \, (e_1p_1)_H \; e'_1>$$

$$= \int d^4y_e \, d^4y_p \, d^4y_{e'} \, d^4x_e \, d^4x_p \, d^4x_{e'} \, \tilde{\mathcal{F}}_{e'}(y_{e'}) \tilde{\mathcal{F}}_{ep}(H, y_e, y_p) \, \sigma(y_e y_p : y_{e'}; x_e x_p : x_{e'})$$

$$\mathcal{F}_{ep}(x_e x_p; H) \mathcal{F}_{e'}(x_{e'}) \qquad (17)$$

It is this last expression that constitutes the starting point of Eden and Rickayzen[4]. We now proceed to calculate the nucleus σ by perturbation theory, corresponding the graphs drawn in Figs.1) and 3), or, more precisely, to the part of those drawings linking all knots. We then have, in an obvious notation:

$$\sigma_{1a} = -e^6 \; \delta(y_{e'}, x_{e'}) \gamma_e^{\mu'} D_{\mu'\nu'} \; (y_e, y_p) \gamma_p^{\nu'} \left\{ \int d^4z_e \; K_F^e(y_e, z_e) \right.$$

$$\left. \gamma_{e'}^{\alpha} \; D_{\alpha\beta}(x_{e'}, z_e) \; \gamma_e^{\beta} \; K_F^e(z_e, x_e) \right\} \gamma_e^{\mu} \; D_{\mu\nu} \; (x_e, x_p) \; \gamma_p^{\nu} \qquad (18a)$$

$$\sigma_{1b} = e^6 \; \delta(y_{e'}, x_{e'}) \; \gamma_e^{\mu'} D_{\mu'\nu'} (y_e, y_p) \gamma_p^{\nu'} \left\{ \int d^4z_p \; K_F^p(y_p, z_p) \right.$$

$$\left. \gamma_{e'}^{\alpha} \; D_{\alpha\beta}(x_{e'}, z_p) \; \alpha_p^{\beta} \; K_F^p(z_p, x_p) \right\} \; \gamma_e^{\mu} \; D_{\mu\nu}(x_e, x_p) \; \gamma_p^{\nu} \qquad (18b)$$

$$\sigma_{1b} = -e^6 \; K_F^e(y_{e'},x_e)\gamma_e^\mu \; D(x_e,x_p) \; \gamma_p^\nu \; K_F^p(y_p,x_p) \; \gamma_e^{\mu'} D_{\mu'\nu'}(y_e,y_p)\gamma_p^{\nu'}$$

$$K_F^e(y_e,x_e) \; \gamma_{e'}^\alpha \; D_{\alpha\beta}(x_e,y_{e'}) \; \gamma_e^\beta \tag{18c}$$

$$\sigma_3 = e^4 \; \delta(y_e,x_{e'}) \; \gamma_e^{\mu'} \; D_{\mu'\nu'}(y_e,y_p)\gamma_p^{\nu'} \; K_F^p \; (y_p,x_p)\gamma_e^\mu \; D_{\mu\nu}(x_p,x_e)$$

$$\gamma_p^\nu \; \delta(y_{e'},x_e) \tag{18d}$$

We shall now concentrate on this last contribution, since the former three can be found in Eden and Rickayzen[(4)] .

If we introduce σ_3 in Eq. 14), and use the Bethe Salpeter in its ladder form for QED we arrive at

$$<(e_2p_2)_H \; e'_2 \; |S-1| \; (e_1p_1)_H \; e'_1> =$$

$$= \int d^4 \, y_e \; d^4 \, y_{e'} \; d^4x_p \; d^4x_e \; d^4x_{e'}$$

$$\tilde{\mathfrak{F}}_e(y_{e'})\tilde{\mathfrak{F}}\,(y_e \; y_p; \; H)K_F^{e^{-1}}(x_e,y_e)K_F^{p^{-1}}(y_p,x_p)$$

$$\mathfrak{F}(x_ex_p;H)\,\mathfrak{F}_{e'}(x_{e'}) \tag{19}$$

*Going into momentum space we need the following representations

$$\mathfrak{F}_{ep}(x_1x_2;H) = \exp\left\{ -i \; P(\mu_ex_1+\mu_px_2)\right\} \; (2\pi)^{-4}$$

$$\int d^4p_r \; \exp\left\{-i \; p_r(x_1-x_2)\right\}\Psi_n(p_r)$$

$$\mathfrak{F}_e(x) = \Psi_e(k) \; e^{-ikx}$$

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*Notice that Eq.(19) is true in a more general framework than QED perturbation theory. In fact, it will subsequentely appear that one would obtain the result of Blankenkecler et al.[(8)] for the proton pole in n-d scattering with $\mu_e = m(m+M)^{-1}$, $\mu_r = M(m+M)^{-1}$, and P and p_r turn out to be the total and relative four momenta of the particles in the hydrogen atom. For $|K_F^i|^{-1}$ we use the usual representation and after performing some trivial integrations we get:

$$< (e_2 p_2)_H \, e_2' \; |S-1| \; (e_1 p_1)_H \, e_1' >=$$

$$=< e(p_e') \; H(P') \; |S-1| e(p_e) \; H(P) >$$

$$= i(2\pi)^4 \delta(P' + p'_e - P - p_e) \overline{\Psi}(p_e') \overline{\Psi}_H(p_e - \mu_e P') (\not{p}_e - m)$$

$$(\not{P} - \not{p}_e' - M)(\not{p}_e' - m) \; \overline{\Psi}_H(p_e' - \mu_e P) \; \Psi(p_e) \qquad (20)$$

Notice that in Eqs.(19) and (20) we have the Dirac operator operating on free particle spinors. We shall show next that they don't do any harm. Remark that the only approximation up to now has been the use of the general ladder approximation (without the instaneous limit).

If we now go into the non-relativistic limit, in the laboratory system,

$$P \equiv (M_H, \vec{0})$$

$$P' \cong \left(M_H + 0 \left(\frac{p_e^2}{M} \right) , \vec{\Delta} \right)$$

The relation between the solution $\Psi_H(p_r)$ of the Bethe-Salpeter equation and the solution of the non-relativistic Schrödinger equation is, following Salpeter[10]:

$$\Psi_H(p) = -(2\pi i)^{-1}\{W - E_e(p)\}\{m - E_e(\vec{p}) + p_4 + i\delta\}^{-1}$$

$$\{W - m - p_4 + i\delta\}^{-1}\phi_s(\vec{p}) \qquad (21)$$

with $\qquad W = m - \varepsilon$

In our case, for instance,

$$E_e(\vec{p}) = |(\vec{p}_e' - \mu_e\vec{P})^2 + m^2|^{1/2} = |\vec{p}_e'^2 + m^2|^{1/2}$$

$$p_{r_4} = E_e' - M_H \cdot m\ (m+M) \cong E_e' - m + \varepsilon\frac{m}{M} + 0\left(\left(\frac{m}{M}\right)\right)^e$$

and we see that in the limit as $M \to \infty$ a zero appears in the first denominator of (21) that cancels the apparent zero of the numerator for the ingoing free electron. This is not, however a property of the limit, as may be shown by using the procedure of Blankenbecler et al[8] or considering the relationship of a vertex function and the relativistic wave function for a bound state.

The final result that obtains is, in the limit $M \to \infty$:

$$\langle e(p_e')\ H(P')\ |S-1|\ e(p_e)\ H(P)\rangle =$$

$$= -i(2\pi)^2\,\delta(P' + p_e' - P - p_e)\ \phi_s^*(\vec{p}_e)\ \Psi_e(\vec{p}_e')\,(\not{P} - \not{p}'_e - M)$$

$$\Psi_e(\vec{p}_e)\ \phi_s(\vec{p}_e) \qquad (22)$$

Notice that the three momenta of the external electrons became relative momenta of non-relativistic hydrogen atom wave functions (recall Eq.(5)).

Upon introducing the correct normalizations

$$\Psi_e(\vec{p}) = (2\pi)^{-3/2}\ m^{1/2}$$

$$\phi_s(\vec{p}) = \pi^{1/2}\ (4a)^{3/2}\ (1 + \vec{p}^2\ a^2)^{-2}$$

with a the Born radius

$$a = (m\ e^2)^{-1}$$

and calculating

$$\not{P} - \not{p}_e' - M \simeq P_0 - E_e' - M \simeq -\left(\varepsilon + \frac{\vec{p}'^2}{2m}\right)$$

$$= -\frac{e^2}{2a}\ (1 + \vec{p}_e^2\ a^2) \qquad \left(|\vec{p}_e'| = |\vec{p}_e| + 0\left(\frac{1}{M}\right)\right)$$

Eq.(22) reduces to the result

$$\langle e(p_e')H(P')\ |S-1|\ e(p_e)H(P)\rangle = i\ 16\ a\ \ \delta(P' + p'_e - P - p_e)$$

$$(1 + p_e^2\ a^2)^{-3} \qquad (23)$$

This, as taken above, is the Born term for electron-proton potential with exchange in the scattering of electrons off hydrogen atoms. Notice that the singularity results from the hydrogen wave function. Were the potential a short range one, we would obtain a simple pole, as is normal in S-matrix theory.

3. SUMMARY, CONCLUSIONS AND DISCUSSION

We have given a systematic procedure to calculate perturbatively the scattering of electrons by hydrogen atoms (and possibly other composite targets) starting from the full relativistic quantum theory, and to obtain its non-relativistic limit keeping under close control the approximations made. The procedure is not limited to electromagnetic interactions neither to the perturbative calculation. It condenses a number of results scattered in the literature, although it is not new and comes from the application of the ideas of Nishijima[9]. It may prove useful to calculate contributions needed in the application of dispersion relations to electron-atom scattering.[11]

When applied to the exchange of a proton, in the sense of Figure **2**, in electron-hydrogen atom scattering it allows to show the identity of this contribution and the exchange Born term in the non relativistic limit for the electron-proton potential contribution. A triple pole results from the long-range forces, as distinct from the simple pole obtained with short range forces. Moreover, the singularity is a dominant one for the process, providing, as is well known, an exceedingly large contribution at very low energies. Another interesting feature is the fact this contribution and its first order radiative correction, the exchange electron-electron potential Born term, are on the same footing. This looks similar to the problem of identifying contributions to radiative corrections in bound Coulomb systems.

A number of applications seem to open, especially in atomic scattering for processes where an electron may be exchanged (p-H, H_e^+ - H_e scattering, etc) and are currently under study.

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FIGURE CAPTIONS

Figure 1 - Diagrammatic description of contributions to electron-hydrogen atom scattering. Straight lines correspond to charged massive particles, wiggly lines to photons and the striped bands represent the bound (hydrogen atom) state. Large dots indicate the usual interaction vertices of quantum electrodynamics. Same conventions are adopted in figures 2 and 3.

Figure 2 - Feynman diagrams contributing to the case of a proton first interacting exclusivelly with one electron and then interacting exclusively with the other.

Figure 3 - Diagram describing the exchange of the proton between the two electrons in the collision between an electron and a hydrogen atom. It may be understood as the sum (in the bound state theory sense) of the Feynman diagrams of Figure 2.

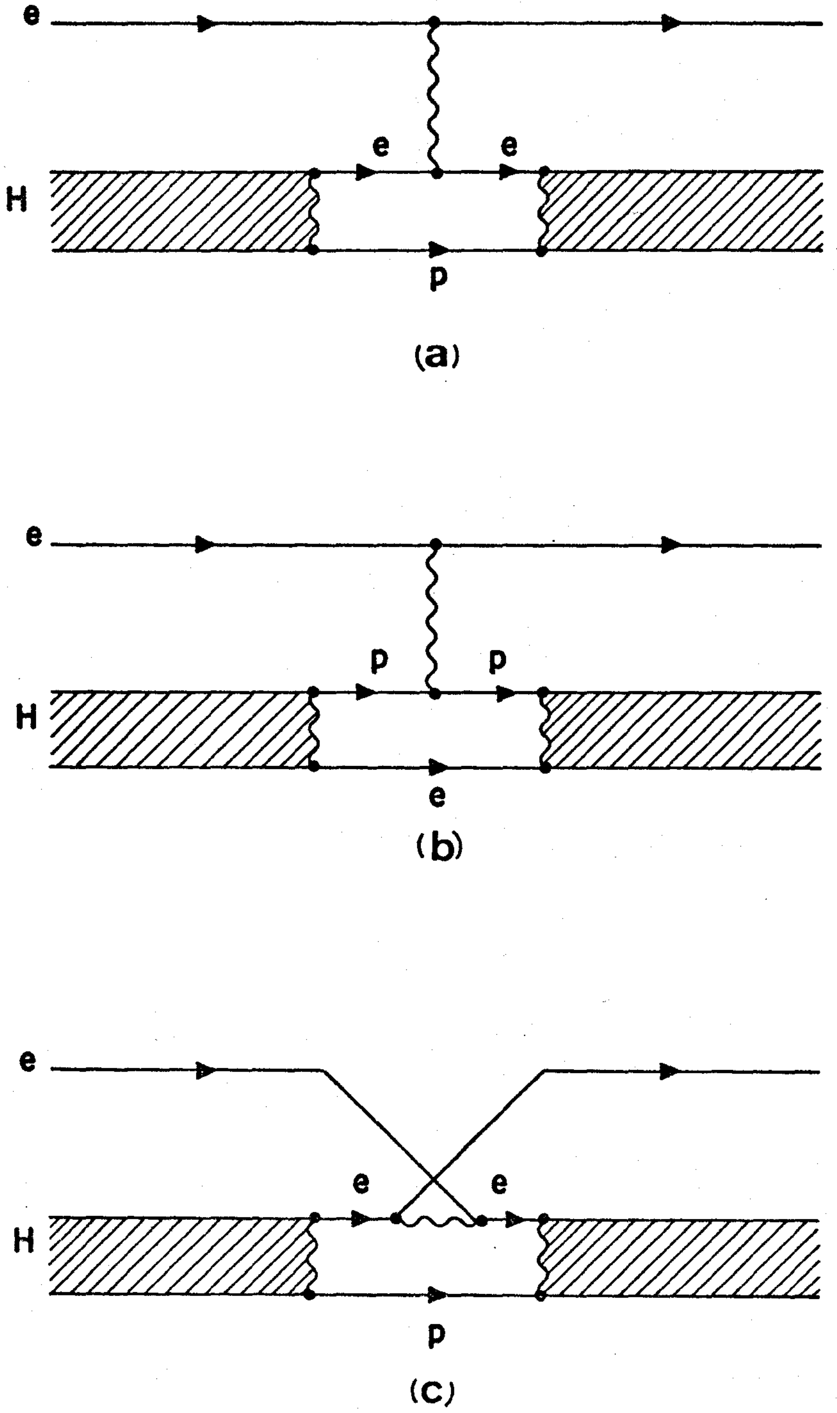

FIG. 1

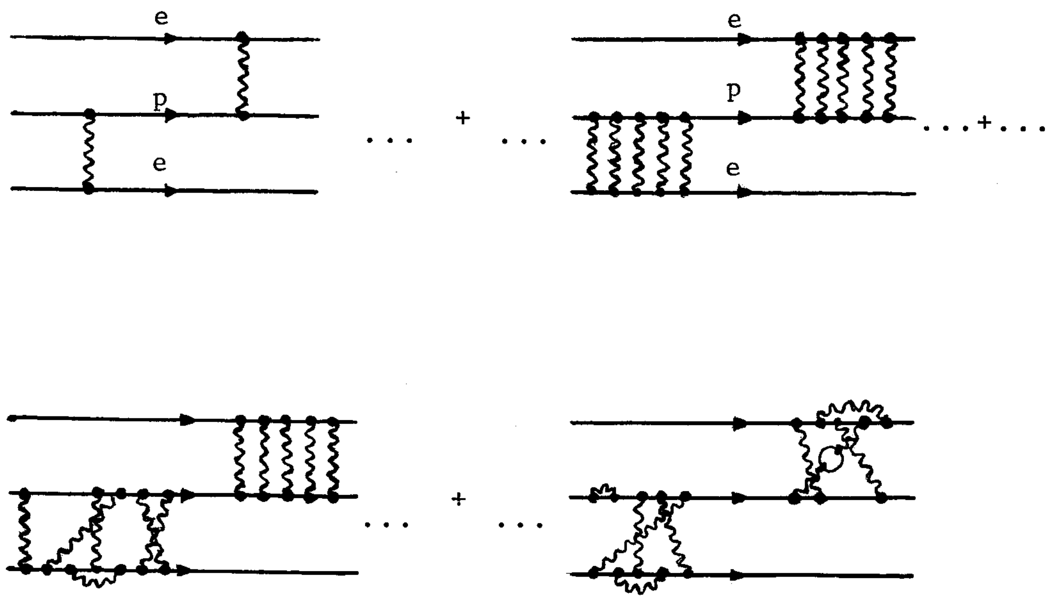

Fig. 2

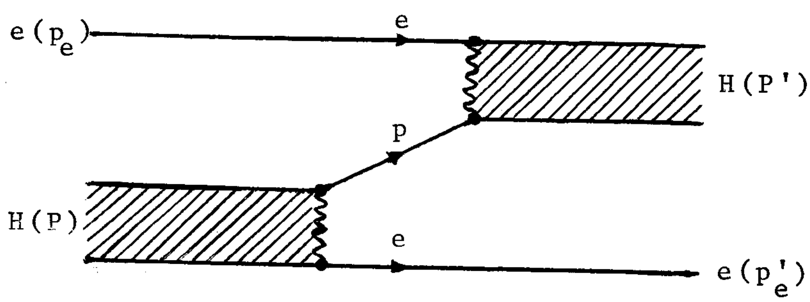

Fig. 3