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Potential scattering in Dirac field theory

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Abstract We develop the potential scattering of a spinor within the context of perturbation field theory. As an application, we reproduce, up to second order in the potential, the diffusion results for a potential barrier of quantum mechanics. An immediate consequence is a simple generalization to arbitrary potential forms, a feature not possible in quantum mechanics.

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1 Introduction

Quantum field theory and the consequent renormalization theory has had unparalleled success [1–3]. However, many calculations in the physics literature are based upon one-particle equations in quantum mechanics [4–6]. This is not simply because quantum field theory calculations are, in general, more cumbersome than quantum mechanical calculations. The real reason is principally the method of calculation. Quantum field theory calculations are often limited by the use of a perturbation approach which can rarely be summed. For example, quantum field theory successfully predicts the Lamb shift [7] but, to the best of our knowledge, there is no direct calculation of the hydrogen atom in field theory. Bound states are almost exclusively treated in quantum mechanics [8]. From quantum field theory one has, at best, the two-body equations, based upon ladder diagrams, such as the Bethe–Salpeter equation [9, 10]. It is even problematic to prove the *mere* existence of some bound states in quantum field theory [11, 12], to discuss the space-time operator in collision descriptions [13, 14] or to analyze the kinematics of spinning particle [15–18]. Another example is that of potential scattering. Many important phenomena such as tunneling [19–24], multiple diffusion [25, 26], and the Klein paradox [27–31], to mention but a few, are described in quantum mechanics be it with the Schrödinger, Klein–Gordon or Dirac equation. Must one be limited for the description of these phenomena to quantum mechanics? Are the quantum mechanical results exact? Generally, experiment answers our doubts, but this is not always feasible.

In this paper, we intend to propose a field theoretic study of potential scattering, one of the mainstays of quantum mechanics. First, we write down the potential interaction term for the Dirac Lagrangian. This is followed by an outline of the quantum field theory treatment of this system. We then apply the perturbation series to a specific potential, that of a single one-dimensional barrier, impinged upon perpendicularly by an incoming momentum eigenstate. We calculate the lowest order contributions and compare them with a Taylor expansion of the expressions for transmission and reflection amplitudes for above barrier diffusion, obtained with the Dirac equation [26]. We can in this way determine if there are any discrepancies between quantum mechanics and quantum field theory calculations and directly test our quantum field theory approach.

In the next section, we present the quantum field theory formalism [3]. In Sect. 3, we calculate the zeroth and first order terms. In Sect. 4 we derive, in some detail, the calculation of the second order terms. Our results are compared with those of the Dirac equation in Sect. 5. We conclude in that section with a discussion of our results.

2 Formalism

The first-quantized quantum mechanical equation for a Dirac spinor involving a time-independent one-dimensional potential $V(x_3)$ is given by

$$(i\partial\!\!\!/ - m)\psi(x) = V(x_3)\gamma_0\psi(x), \tag{1}$$

where $x = (t, \boldsymbol{x})$. Actually, the above choice $V\gamma_0\psi$ is for an *electrostatic* potential, since it can be derived from a

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four-vector potential interaction $A_\mu \gamma^\mu \psi$, when $\boldsymbol{A} = 0$ and $A_0 = V$. An alternative and generally non-equivalent choice would be the *scalar* interaction $V\psi$. In standard field theory the two choices imply spinors interacting through the exchange of vector and scalar particles. However, in contrast to standard field theory, we shall not second-quantize this potential field. Throughout this paper V will be a (c-number) function. This allows us to compare our results directly with those of the Dirac equation.

From (1), which is equally valid for the Dirac field, we immediately derive the following Lagrangian density:

$$\mathcal{L}(x) = \overline{\psi}(x)(i\partial\!\!\!/ - m)\psi(x) - V(x_3)\overline{\psi}(x)\gamma_0\psi(x). \tag{2}$$

The spinor field can be quantized in the standard way. In the interaction picture, the resulting spinor field takes the well-known form

$$\psi(x) = \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3 2E(\boldsymbol{k})} \times \sum_s \left[a^s_{\boldsymbol{k}} u^s(\boldsymbol{k}) e^{-ikx} + b^s_{\boldsymbol{k}} v^s(\boldsymbol{k}) e^{ikx}\right], \tag{3}$$

where $k = [E(\boldsymbol{k}), \boldsymbol{k}]$, $E(\boldsymbol{k}) = \sqrt{\boldsymbol{k}^2 + m^2}$ and $kx = E(\boldsymbol{k})t - \boldsymbol{k}\cdot\boldsymbol{x}$. Technically, the time dependence of the field is a consequence of working in the interaction picture and the assumption of anti-commutators for creation/annihilation operators.

The S-matrix for any process is formally given by

$$\langle \mathrm{out}|S|\mathrm{in}\rangle = {}_0\langle \mathrm{out}|T\left\{\exp\left[-i\int \mathrm{d}^4x \mathcal{H}_{\mathrm{int}}(x)\right]\right\}|\mathrm{in}\rangle_0, \tag{4}$$

where T means time-ordered. In the above, it is understood that only connected terms are to be considered and the incoming and outgoing states are defined by the action of creation operators upon the free field vacuum state (indicated by the subscript 0). For an excellent derivation of the above we refer the reader to the book of Peskin and Schroeder [3]. From (2), we see that

$$\mathcal{H}_{\mathrm{int}}(x) = V(x_3)\overline{\psi}(x)\gamma^0\psi(x). \tag{5}$$

Equation (4) can be evaluated by expanding in powers the interaction Hamiltonian within the time-ordered integral. This is the basis of the perturbation approach. Normally, the unit (0th order) term is neglected and one considers only the so-called T-matrix. However, for our purposes we start by re-deriving this unit term since it must reproduce the transmission amplitude of the Dirac equation in the limit of *zero* potential.

We choose the incoming state to be a spinor of mass m travelling along the x_3 axis,

$$\boldsymbol{p} = (0, 0, p_3), \qquad E(\boldsymbol{p}) = \sqrt{p_3^2 + m^2} := E,$$

with unspecified spin s. The outgoing state can only be a spinor of mass m, the only mass in the Lagrangian, to which we assign an arbitrary spin r and momentum $\boldsymbol{p}'$. As we shall prove in the following sections, only the values with $r = s$ and $\boldsymbol{p}' = (0, 0, \pm p_3)$ contribute, corresponding to spin conserving transmission and reflection.

3 Zeroth and first order contributions

Our objective is to calculate in field theory the transmission and reflection *amplitude* defined in quantum mechanics. This involves some significant difference when compared to other field theory calculations.

The first term in the expansion of (4) is simply given by

$${}_0\langle \boldsymbol{p}', r|\boldsymbol{p}, s\rangle_0 = 2E(2\pi)^3\delta^3(\boldsymbol{p}' - \boldsymbol{p})\delta_{rs}. \tag{6}$$

This must correspond to the unit contribution of a non-interacting quantum mechanical particle. Thus, we see that the above result has to be integrated over the final three-momentum $\boldsymbol{p}'$ and specifically with the standard relativistically invariant measure,

$$\int \frac{\mathrm{d}^3\boldsymbol{p}'}{(2\pi)^3 2E(\boldsymbol{p}')} \langle \boldsymbol{p}', r|\boldsymbol{p}, s\rangle_0 = \delta_{rs}. \tag{7}$$

However, it is important to note that this results yields a non-zero contribution only for $\boldsymbol{p}' = \boldsymbol{p}$, i.e. for transmission, as required. The explicit Kronecker delta reminds us that there is no spin flip contribution. This delta is sometimes not written in the literature but expressed in words. In this paper we shall, instead, display it explicitly, even though it will be a common factor throughout. Summing over the final spin is seen not to be advisable since it would lose information.

Consequent to the above discussion all our field theoretic terms will henceforth be integrated over the final state momentum, but not summed over final state spins. It is a little unusual to do final state momentum integrations before squaring the amplitude as occurs in the calculation of cross sections and decay rates. However, a positive aspect is that it avoids the encounter of the square of delta functions and the subsequent need to define rates per unit time and unit volume. Actually, the final state momentum integration will never be completed. We will always separate (and not add) the transmitted and reflected contributions. Other unusual features compared to standard field theory calculations are that the final state can only be a single outgoing particle and that three-momentum is not conserved because of reflection.

For the first order term, we must calculate

$$-i{}_0\langle \boldsymbol{p}', r|T\left[\int \mathrm{d}^4x V(x_3)\bar{\psi}(x)\gamma^0\psi(x)\right]|\boldsymbol{p}, s\rangle_0. \tag{8}$$

The fields $\overline{\psi}$ and ψ must be contracted with the outgoing and incoming states, yielding, after adding final state momentum integration

$$-i\int \frac{\mathrm{d}^3\boldsymbol{p}'}{(2\pi)^3 2E(\boldsymbol{p}')}\,\mathrm{d}^4x \times V(x_3)\langle 0|u^{r\dagger}(\boldsymbol{p}')e^{i(p'-p)x}u^s(\boldsymbol{p})|0\rangle. \tag{9}$$

Performing the space-time integrals, with the exception for the coordinate x_3, and the transverse outgoing momentum integrals, we obtain

$$-i\int \frac{\mathrm{d}p_3'}{4\pi E}\,\mathrm{d}x_3 V(x_3)\delta(E'-E) \times \exp\bigl[-i(p_3'-p_3)x_3\bigr]\langle 0|u^{r\dagger}(p_3')u^s(p_3)|0\rangle, \tag{10}$$

where $E'=\sqrt{{p_3'}^2+m^2}$. For the integration over the third component of the momentum, we use the identity

$$\delta(E'-E)=\frac{E}{p_3}\bigl[\delta(p_3'-p_3)+\delta(p_3'+p_3)\bigr].$$

Thus, in the amplitude there will be two incoherent contributions. One for $p_3'=p_3$ (transmission) and one for $p_3'=-p_3$ (reflection). These must be treated separately. For transmission, we find

$$-\frac{i}{2p_3}\langle 0|u^{r\dagger}(p_3)u^s(p_3)|0\rangle\int \mathrm{d}x_3 V(x_3) = -i\frac{E}{p_3}\int \mathrm{d}x_3 V(x_3)\delta_{rs}, \tag{11}$$

while, for reflection, we obtain

$$-\frac{i}{2p_3}\langle 0|u^{r\dagger}(-p_3)u^s(p_3)|0\rangle\int \mathrm{d}x_3 V(x_3)\exp[2ip_3x_3] = -i\frac{m}{p_3}\int \mathrm{d}x_3 V(x_3)\exp[2ip_3x_3]\delta_{rs}. \tag{12}$$

We must now perform the x_3 integrals. To do so, we must now select a specific potential. We apply our formalism to a *barrier* potential of height V_0 and situated on the x_3 axis between 0 and L,

$$V(x_3)=\{0\ (x_3<0),\ V_0\ (0<x_3<L),\ 0(x_3>L)\}.$$

The results of the elementary x_3 integrations are

$$-i\frac{E}{p_3}V_0L\delta_{rs} \tag{13}$$

for transmission, and

$$-i\frac{mV_0}{p_3^2}\sin(p_3L)\exp[ip_3L]\delta_{rs} \tag{14}$$

for reflection.

A comment before proceeding to the calculation of the second order terms. Because of the x_3 dependence of the potential V, we cannot perform all of the space-time integrals trivially, and thus we do *not* have overall energy-momentum conservation. However, energy conservation (a consequence of the x_0 integration) together with the mass shell conditions implies the conservation of the square of the three momentum. This means that the allowed contributions are transmission and reflection. There is nothing unusual in this. Even in reflection from a step function only momentum squared is conserved as also for our bound state quantum mechanical problem.

4 Second order contribution

The second order contribution is given by

$$-\frac{1}{2}{}_0\langle \boldsymbol{p}', r|T\biggl[\int \mathrm{d}^4x\,\mathrm{d}^4y V(x_3)V(y_3) \times \overline{\psi}(x)\gamma^0\psi(x)\overline{\psi}(y)\gamma^0\psi(y)\biggr]|\boldsymbol{p},s\rangle_0. \tag{15}$$

The two modes of contraction result in identical contributions and hence simply cancel the factor of $\frac{1}{2}$ above. We are thus left with the calculation of

$$-\int \frac{\mathrm{d}^3\boldsymbol{p}'}{(2\pi)^3 2E(\boldsymbol{p}')}\,\mathrm{d}^4x\,\mathrm{d}^4y V(x_3)V(y_3) \times \langle 0|u^{r\dagger}(\boldsymbol{p}')e^{ip'x}S_{\mathrm{F}}(x-y)e^{-ipy}\gamma_0u^s(\boldsymbol{p})|0\rangle, \tag{16}$$

where $S_{\mathrm{F}}(x-y)$ is the Feynman propagator,

$$S_{\mathrm{F}}(x-y)=\int \frac{\mathrm{d}^4k}{(2\pi)^4}\frac{i(\not{k}+m)}{k^2-m^2+i\epsilon}e^{-ik(x-y)}.$$

Before continuing, we wish to observe that there are eight space-time integrals to perform and seven momentum integrals. Only six space time integrals can be immediately executed yielding six delta functions. These can then be used to integrate over the momenta and specifically over all but the k_3 momentum. Also remaining are the $\mathrm{d}x_3$ and $\mathrm{d}y_3$ integrals. The k_3 momentum will be integrated in the complex plane and the final space integrals by elementary means. During this procedure, we use the treatment described in the previous section for the $\delta(E'-E)$ to perform the $\mathrm{d}p_3'$ integral. This is the point in which separation between transmission and reflection occurs.

The integration over the space-time variables, excluding x_3 and y_3, yields the following delta functions:

$$\delta(p_0'-k_0)\delta(p_1'-k_1)\delta(p_2'-k_2)\delta(p_0-k_0) \times \delta(p_1-k_1)\delta(p_2-k_2).$$

We then integrate over the transverse momenta both for $\boldsymbol{k}$ and $\boldsymbol{p}'$. The integral over $\mathrm{d}k_0$ leaves us with one remaining energy delta function which we rewrite as a sum of delta's in p_3': one delta for transmission and one for reflection. After performing the $\mathrm{d}p_3'$ integral, for transmission, we obtain

$$
\begin{aligned}
&-\int \frac{\mathrm{d}k_3}{4\pi p_3}\,\mathrm{d}x_3\,\mathrm{d}y_3 V(x_3)V(y_3)\exp\bigl[ip_3(y_3-x_3)\bigr]\\
&\quad\times\langle 0|u^{r\dagger}(p_3)\frac{i(\gamma_0 E-\gamma_3 k_3+m)}{p_3^2-k_3^2+i\epsilon}\\
&\quad\times\exp\bigl[ik_3(x_3-y_3)\bigr]\gamma_0 u^s(p_3)|0\rangle, \qquad (17)
\end{aligned}
$$

and for reflection,

$$
\begin{aligned}
&-\int \frac{\mathrm{d}k_3}{4\pi p_3}\,\mathrm{d}x_3\,\mathrm{d}y_3 V(x_3)V(y_3)\exp\bigl[ip_3(y_3+x_3)\bigr]\\
&\quad\times\langle 0|u^{r\dagger}(-p_3)\frac{i(\gamma_0 E-\gamma_3 k_3+m)}{p_3^2-k_3^2+i\epsilon}\\
&\quad\times\exp\bigl[ik_3(x_3-y_3)\bigr]\gamma_0 u^s(p_3)|0\rangle. \qquad (18)
\end{aligned}
$$

The $\mathrm{d}k_3$ integral can be performed with the help of the residue theorem. However, the result is different for $x_3>y_3$ or $x_3<y_3$. According to the case, we must close the contour above or below the axis. We have

$$
\begin{aligned}
&\int \mathrm{d}k_3\frac{i(\gamma_0 E-\gamma_3 k_3+m)}{p_3^2-k_3^2+i\epsilon}\exp\bigl[ik_3(x_3-y_3)\bigr]\\
&\quad=\theta(x_3-y_3)\frac{\pi}{p_3}(\gamma_0 E-\gamma_3 p_3+m)\exp\bigl[ip_3(x_3-y_3)\bigr]\\
&\qquad+\theta(y_3-x_3)\frac{\pi}{p_3}(\gamma_0 E+\gamma_3 p_3+m)\exp\bigl[ip_3(y_3-x_3)\bigr].
\end{aligned}
$$

Whence the second order contribution to transmission, $p_3'=p_3$, reads

$$
\begin{aligned}
&-\frac{1}{4p_3^2}\int \mathrm{d}x_3\,\mathrm{d}y_3 V(x_3)V(y_3)\exp\bigl[ip_3(y_3-x_3)\bigr]\\
&\qquad\times\bigl\{\theta(x_3-y_3)\langle 0|u^{r\dagger}(p_3;E)(\gamma_0 E-\gamma_3 p_3+m)\\
&\qquad\times\gamma_0 u^s(p_3;E)|0\rangle\exp\bigl[ip_3(x_3-y_3)\bigr]\\
&\qquad+\theta(y_3-x_3)\langle 0|u^{r\dagger}(p_3;E)(\gamma_0 E+\gamma_3 p_3+m)\\
&\qquad\times\gamma_0 u^s(p_3;E)|0\rangle\exp\bigl[ip_3(y_3-x_3)\bigr]\bigr\}\\
&\quad=-\frac{1}{p_3^2}\int \mathrm{d}x_3\,\mathrm{d}y_3 V(x_3)V(y_3)\bigl\{\theta(x_3-y_3)E^2\\
&\qquad+\theta(y_3-x_3)m^2\exp[2ip_3(y_3-x_3)]\bigr\}\delta_{rs}. \qquad (19)
\end{aligned}
$$

The second order contribution for reflection, $p_3'=-p_3$, reads

$$
\begin{aligned}
&-\frac{1}{4p_3^2}\int \mathrm{d}x_3\,\mathrm{d}y_3 V(x_3)V(y_3)\exp\bigl[ip_3(y_3+x_3)\bigr]\\
&\qquad\times\bigl\{\theta(x_3-y_3)\langle 0|u^{r\dagger}(-p_3;E)(\gamma_0 E-\gamma_3 p_3+m)\\
&\qquad\times\gamma_0 u^s(p_3;E)|0\rangle\exp\bigl[ip_3(x_3-y_3)\bigr]\\
&\qquad+\theta(y_3-x_3)\langle 0|u^{r\dagger}(-p_3;E)(\gamma_0 E+\gamma_3 p_3+m)\\
&\qquad\times\gamma_0 u^s(p_3;E)|0\rangle\exp\bigl[ip_3(y_3-x_3)\bigr]\bigr\}\\
&\quad=-\frac{mE}{p_3^2}\int \mathrm{d}x_3\,\mathrm{d}y_3 V(x_3)V(y_3)\bigl\{\theta(x_3-y_3)\exp[2ip_3x_3]\\
&\qquad+\theta(y_3-x_3)\exp[2ip_3y_3]\bigr\}\delta_{rs}. \qquad (20)
\end{aligned}
$$

After performing the x_3 integration, we find

$$
-\left\{\frac{E^2L^2}{2p_3^2}+\frac{m^2}{4p_3^4}\bigl(1-\exp[2ip_3L]+2ip_3L\bigr)\right\}V_0^2\delta_{rs}, \qquad (21)
$$

for transmission, and

$$
i\frac{mE}{p_3^4}\exp[ip_3L]\bigl\{p_3L\exp[ip_3L]-\sin(p_3L)\bigr\}V_0^2\delta_{rs}, \qquad (22)
$$

for reflection.

5 Conclusions

In the previous two sections, we have calculated the 0th, 1st and 2nd order contributions of spinor field theory to scattering off a simple one-dimensional barrier. Now, we compare these results with those of quantum mechanics. We recall the full expressions for the Dirac transmission and reflection coefficients [26],

$$
\begin{aligned}
R_{\mathrm{D}}&=-i\frac{mV_0}{q_3p_3}\sin(q_3L)\\
&\quad\Big/\left[\cos(q_3L)-i\frac{p_3^2-EV_0}{q_3p_3}\sin(q_3L)\right], \qquad (23)\\
T_{\mathrm{D}}&=\exp[-ip_3L]\Big/\left[\cos(q_3L)-i\frac{p_3^2-EV_0}{q_3p_3}\sin(q_3L)\right],
\end{aligned}
$$

where $q_3=\sqrt{(E-V_0)^2-m^2}$. We have re-expressed R_{D} in order to explicitly display the V_0 dependence. Polarization conservation in [26] was stated and not given in terms of a Kroneker delta. The first terms of the Taylor expansions in V_0 are

$$
\begin{aligned}
R_{\mathrm{D}}&\approx -i\frac{mV_0}{p_3^2}\sin(p_3L)\exp[ip_3L]\\
&\quad+i\frac{mEV_0^2}{p_3^4}\exp[ip_3L]\bigl\{p_3L\exp[ip_3L]-\sin(p_3L)\bigr\},
\end{aligned}
$$

$$T_{\mathrm{D}} = 1 - i\frac{E}{p_3}V_0 L - \left[\frac{E^2L^2}{2p_3^2} + \frac{m^2}{4p_3^4}\left(1 - \exp[2ip_3L] + 2ip_3L\right)\right]V_0^2. \quad (24)$$

Agreement with our field theory calculations up to and including second order is found. This result was not an obvious prediction, a priori. First, because the calculational methods are very different. Secondly, because while in quantum mechanics continuity plays a major role, in field theory continuity never appears, but antiparticles do; for example they are intrinsic in the Feynman propagator. Furthermore, while for diffusion there are no particular surprises with the quantum mechanical results, this is not true for tunnelling. In tunnelling, it has been shown elsewhere that the Hartman effect exists. This is an apparent violation of causality which we do not expect in any field theory calculation. Indeed, it was one of the original stimuli for developing the above formalism. Unfortunately, our results do not extend into the tunnelling region. However, one of the advantages of the above agreement, which we postulate holds to *all* orders, is that it confirms the correctness of our procedures.

An important consequence of our formalism is that since the potential functions are merely integrated over, the application of our procedures to *any* potential shape is straightforward, and in some cases, when the integrations can be performed analytically, even simple. This is not the case for general step-wise potentials in quantum mechanics. There, the calculational difficulties (coupled matrix equations) grow at least linearly with the number of potential discontinuities.

The perturbation approach is not valid for tunneling. This merits a comment. In quantum mechanics, it is possible to treat tunneling and diffusion simultaneously. The only difference, which can be left to almost the end of the calculation, is that the momentum q_3 is either real (for diffusion) or pure imaginary (for tunneling). This essentially transforms trigonometric functions in hyperbolic functions. However, the problem lies elsewhere. It is that while a factor like $\sqrt{(E-V_0)^2-m^2}$ for $E > V_0 + m$ (diffusion) can be Taylor expanded in V_0, for $E < V_0 - m$ (tunneling) it *cannot*. Of course, if one believes that the tunneling results are an analytic continuation of the diffusion results, our field theory calculation should yield the same tunneling results. However, a place where this is clearly not the case is in the Klein energy zone. The Klein paradox for a step potential is interpreted as the creation at the potential discontinuity of particle–antiparticle pairs. This is obviously inconsistent with the single particle nature of the Dirac equation, but has been seen as an anticipation of field theory. The characteristic of this paradox is a reflection coefficient greater than one. If one treats the barrier potential, in the Klein zone, in the standard way, one finds instead *no* paradox. Recently, a pair creation treatment of the barrier has been provided [31]. It implies the existence of a new type of spatial localization, since the antiparticles created at each reflection are necessarily blocked within the barrier, which they see as a potential well. So, what more appropriate a subject for a field theoretical treatment than the Klein zone of the barrier. At the moment, this remains a feature objective.

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