Dirac Equation : Wave Function and Phase Shifts for a Linear Potential

Lalit K. Sharma*, and Lesolle D. Sebitla
Department of Physics, University of Botswana, P/Bag 0022, Gaborone, Botswana.
*Author for correspondence, e-mail: sharmalk@mopipi.ub.bw

ABSTRACT

In this paper, we derive the asymptotic expressions for the wavefunctions and s-wave phase shifts for a linear potential in the Dirac equation. The presentation is done from the two coupled equations for the radial parts of the Dirac equation. A simple method for correcting the above obtained expressions has also been discussed. This expression has been found to provide good results for small values of r.

Keywords : Dirac equation, s-wave phase shifts, and wavefunction.

1. INTRODUCTION

Investigations on the intense electron beams [1] and the presence of other configurations of parallel electric and magnetic fields [2] in astrophysical problems, in which relativistic particles possibly exists [3], have led to the necessity for a clear understanding of relativistic quantum particles in an external electromagnetic fields and their scattering problems. This can readily be accomplished if we know the exact solutions to the Dirac equation. Sharma and Fiase [4] and Wen-Chao [5] have presented the exact solutions for the electromagnetic potentials which assumed a particular functional dependence on the space coordinates. A careful literature survey reveals that very few solvable configurations which have exact solution have been found since the formulation of the Dirac equation. The important solutions are for the constant magnetic field [6], constant electric field [7] and the Coulomb potential [8].

Scattering problems have been discussed by many authors [9-13] for non-relativistic particles and corresponding expressions for the phase shifts have been derived. In the course of investigating problems on scattering of high energy electrons with heavy nuclei, a number of results for the relativistic cases were obtained. Tietz [14], Sharma, et al. [15] and Parzen [16] derived expressions of the phase shifts for Dirac equations. Sharma et.al.,[15] applied Wronskian methods for deriving phase shifts in the case of Klein-Gordon and Dirac particles. Conditions in the non-relativistic limit have also been discussed by him. Parzen [16] has derived the phase shift expression by a variational principle. This expression is found to be more accurate than the corresponding expression obtained by the Born approximation for strong potentials at very high energies.

Rose [17] obtained the asymptotic expression for the phase shift by the WKB treatment. Based on the work of Sharma et.al.,[15] and Good [8]. Shunqing and Ruibao [18] re-derived Rose’s [17] form of asymptotic expression in a different way for the Coulomb potential. This derivation permits a quantitative
estimate to be made of the error in the WKB approximation in a perturbative manner. The expression of Shunquing and Ruibao \[18\] is found to be quite accurate even for small values of \(r\).

In this paper expressions for the wavefunction and s-wave phase shifts have been derived for a linear coulomb potential in the Dirac equation. Corrections to the phase shifts have also been calculated.

2. THE ASYMPTOTIC WAVEFUNCTION FOR THE LINEAR COULOMB POTENTIAL

The two coupled equations for the radial parts of the Dirac equation can be presented

\[
\frac{dF}{dr} - \frac{K}{r} \frac{V - E - mc^2}{\hbar c} G = 0 \tag{1}
\]

\[
\frac{dG}{dr} + \frac{K}{r} \frac{G - V - E + mc^2}{\hbar c} F = 0 \tag{2}
\]

with the parameter \(K\) defined as:

\[
K = \pm (j + 1/2) \text{ for } l = j \pm 1/2
\]

where \(l\) is the orbital angular momentum designation in the non-relativistic nomenclature, and \(E\) the energy and that \(E > mc^2\). We now proceed to rederive the Rose’s form \[17\] of asymptotic expression of equations (1) and (2) by different procedure. This derivation not only enables the quantitative estimation of the error involved in the WKB approximation but also improves systematically the approximation perturbatively.

Now setting

\[
F = (\hbar c)^{-1/2} A(E - V + mc^2)^{1/2} \left(\frac{d}{dr}\right)^{-1/2} \cos \varphi \tag{3}
\]

(A being a constant)
in the Dirac equation (1) and (2), one finds \(\varphi\) to satisfy the following nonlinear equation

\[
-\left(\frac{d\varphi}{dr}\right)^2 + \frac{(E - V)^2 - m^2 c^4}{\hbar^2 c^2} - \frac{K(K-1)}{r^2} + \left(\frac{d\varphi}{dr}\right)^{1/2} \frac{d^2}{dr^2} \left(\frac{d\varphi}{dr}\right)^{-1/2} \tag{4}
\]

\[
- (E - V + mc^2)^{1/2} \frac{d^2}{dr^2} (E - V + mc^2)^{-1/2} - \frac{K}{r} \frac{dV/dr}{E - V + mc^2} = 0
\]

Thus equation (3) can be taken as an exact solution of the Dirac equations. A very good approximate solution to equation (4) is obtained by neglecting the last three terms of equation (4) and setting

\[
\left(\frac{d\varphi}{dr}\right)^2 \equiv \frac{(E-V)^2 - m^2 c^4}{\hbar^2 c^2} - \frac{K(K-1)}{r^2} \tag{5}
\]
The approximation of equation (5) yields the WKB approximation in which some very small relativistic terms are neglected. From equation (5), we have

\[ \varphi'(r) = \varphi(r) - \varphi(r_0) = \int_{r_0}^{r} \frac{d\varphi}{dr} dr = \int_{r_0}^{r} \frac{dr}{\hbar c} \left[ (E - V)^2 - m^2 c^4 - \frac{\hbar^2 c^2 K(K-1)}{r^2} \right]^{1/2} \]  

(6)

This equation is solved both numerically and analytically. The values so obtained are shown in Table 1. Equation (6) can also be written as:

\[ \varphi(r) = \varphi(r_0) + \chi(r) - \chi(r_0) \]  

(7)

where

\[ \chi(r) - \chi(r_0) = \int_{r_0}^{r} \frac{dr}{\hbar c} \left[ (E - V)^2 - m^2 c^4 - \frac{\hbar^2 c^2 K(K-1)}{r^2} \right]^{1/2} \]  

(8)

The asymptotic form of the large and small radial wavefunctions may be written with the help of equation (1), (3) and (5). Thus

\[ F \approx \frac{A(E - V + mc^2)^{1/2}}{[(E - V)^2 - m^2 c^4 - \hbar^2 c^2 K(K-1)/r^2]^{1/4}} \cos \varphi \]  

(9a)

and

\[ G = \frac{\hbar c}{(E - V + mc^2)} \left( \frac{dF}{dr} - \frac{K}{r} F \right) \]  

(9b)

We now consider the linear potential of the form:

\[ V = g r \]  

(10a)

In order to avoid the potential going to infinity, we put a restriction such that

\[ r_0 \leq r \leq R \]  

(10b)

where both \( r_0 \) and \( R \) the lower cut-off as well as the upper cut-off points assume only finite values. Substitution of this potential in equation (8) yields for small values of \( r_0 \) and \( K = 0 \),

\[ \chi(r) = \frac{1}{\hbar c} \left[ \frac{2\gamma x + \beta}{4\gamma} \sqrt{R} + \frac{4\alpha x - \beta^2}{8\gamma^{3/2}} \ln(2\sqrt{R} + 2x + \beta) \right] \]  

(11)

In equation (11),

\[
\begin{aligned}
R &= \alpha + \beta x + \gamma x^2 \\
\alpha &= E^2 - m^2 c^4 = \hbar^2 c^2 k^2 \\
\beta &= -2E \\
\gamma &= 1 \\
and \\
x &= gr
\end{aligned}
\]  

(12)
Table 1. Phase Discrepancy \((\phi'_n - \phi'_a)\) between Numerical solution and Asymptotic Solution of equation (6) and Correction \((\Delta \phi)\) to Phase Integral of equation (6).

\[
(g = 1/e^2, \hbar = c = 2m = 1)
\]

<table>
<thead>
<tr>
<th>(g)</th>
<th>(\omega(eV))</th>
<th>(r_0(\text{Å}))</th>
<th>(r(\text{Å}))</th>
<th>(\phi'_n - \phi'_a)</th>
<th>(\Delta \phi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5</td>
<td>1.0</td>
<td>10</td>
<td>0.0038</td>
<td>0.00238</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td>2.5</td>
<td>10</td>
<td>0.0210</td>
<td>0.01320</td>
</tr>
<tr>
<td>1</td>
<td>15</td>
<td>1.0</td>
<td>10</td>
<td>0.4170</td>
<td>0.10410</td>
</tr>
</tbody>
</table>

This expression (11) is valid only for \(R > 0\). \(R\) becomes negative for very small values of \(r\). Further, for very large values of \(r\), equation (11) therefore simplifies to:

\[
\chi(r) \to \frac{1}{ghc} \left[ \frac{1}{2} x \sqrt{\beta x + y x^2} + \frac{4 \alpha y - \beta^2}{8 \gamma^{3/2}} \ln(2 \sqrt{\beta x + y x^2} y + 2 y x) \right] + \delta_0 \tag{13}
\]

where \(\delta_0\) is a constant.

Using equations (7) and (13), we obtain the following expression for \(\delta_0\), the s-wave phase shift:

\[
\delta_0 = \phi(r_\infty) - \frac{1}{ghc} \left[ \frac{x}{2} \sqrt{\beta x + y x^2} + \frac{4 \alpha y - \beta^2}{8 \gamma^{3/2}} \ln(2 \sqrt{\beta x + y x^2} y + 2 y x) \right] \tag{14}
\]

3. ESTIMATION OF THE NEGLECTED TERMS

In equation (4), we have neglected three terms. By substitution of potential \(V\), we found that the contribution of these terms for any value of \(g\), the coupling constant, \(E\) the energy and \(r\) the separation distance is very small compared to the contribution of equation (5).

The following approximations are made for obtaining useful expressions for the size of the neglected terms in equation (4) relative to the term of equation (5):

\[
\frac{E}{\hbar c} \approx \frac{mc}{\hbar} \tag{15}
\]

and

\[
k^2 \approx \frac{E^2 - m^2 c^4}{\hbar^2 c^2} \approx \frac{2m\omega}{\hbar^2} \tag{16}
\]

where

\[
\omega = E - mc^2 \tag{17}
\]

Now for obtaining the error produced in equation (6), we write equation (5) (which gives a lowest order expression) as \(\frac{d\phi_0}{dr}\). Thus the inclusion for the next order gives
where \( E \) is the sum of the three neglected terms. The corresponding correction in the phase integral is given by:

\[
\Delta \varphi = \theta (r) - \theta (r_0) = \frac{1}{2} \int_{r_0}^{r} \frac{d\varphi_0}{dr} \, dr
\]

(19)

The contributions to \( \varphi \) and \( \epsilon \) are again separated into three terms. The smallest term is not treated and the large terms are:

\[
\theta_1 (r) = \frac{r}{R^{3/2}} A + \frac{B}{R^{3/2}} + \frac{r}{R^{3/2}} D + \frac{F}{R^{3/2}}
\]

(20)

where

\[
A = \left[ \frac{5b'c'}{2q} - \frac{5b^2}{12q} - \frac{5g^4}{16c'} + \frac{5g^4b^2}{48c'q} \right],
\]

\[
B = \left[ -\frac{5b^3}{48q} - \frac{5bg^2}{24c'} - \frac{5b^3g^2}{24qc'} + \frac{5g^6b}{96c'^2} + \frac{5g^4b^3}{96qc'^2} \right],
\]

\[
D = \left[ -\frac{5b^3c'}{3q^2} - \frac{10b^3g^2c'}{3q^2} + \frac{5g^4b^3}{6q^2} - \frac{g^2c'}{q} \right],
\]

and

\[
F = \left[ \frac{5b'c'}{6q} - \frac{5b^2}{3q^2} - \frac{5g^4b^3}{12q^2} - \frac{g^2b}{2q} \right]
\]

(21)

Similarly

\[
\theta_2 (r) = -\frac{3hc}{8} \sqrt{X} \left( \frac{(b-2Pc')}{2(a-bP+c'P^2)^{3/2}} \ln \left( \frac{\sqrt{2(a-bP+c'P^2)}X}{2(a-bP+c'P^2)^{3/2}} \right) \right)
\]

(22)

\[
X = c' + (b-2Pc')t + (a-bP+c'P^2)t^2
\]

\[
P = (E + mc^2) / g
\]

(23a)

and

\[
t = \frac{1}{(r + P)}
\]

(23b)

In equation (20) and (22), we have that:

\[
R = a + br + c'r^2
\]

\[
a = E^2 - m^2c^4 = 2m\alpha c^2
\]

\[
b = -2Bq
\]

\[
c' = g^2
\]

\[
q = 4\alpha c^2 - b^2
\]

(24)
The corrections to the phase shift $\delta_0$ of equation (13), introduced by $\Delta \varphi$ are:

$$\lim_{r \to \infty} \theta_1(r) - \theta_1(r_0) = \frac{rA}{a^{3/2}} + \frac{B}{a^{3/2}} + \frac{D}{a^{1/2}} + \frac{F}{a^{1/2}} - \theta_1(r_0)$$

and

$$\lim_{r \to \infty} \theta_2(r) - \theta_2(r_0) = -\frac{3hc}{8} \left[ \frac{\sqrt{c'}}{a-bP+c'P^2} \right] - \theta_2(r_0)$$

Figure 1. Variation of s-wave phase shift ($\delta_0$) with $k^2$ in Angstroms (Å).
4. CONCLUSIONS AND THE INTERPRETATION OF THE GRAPH

In this paper, we have solved equation (6) both numerically and asymptotically. The differences between phases of the two solutions are given in Table 1. The reason for this difference may be ascribed to the neglected terms in equation (4). These values of the neglected terms are calculated from equation (20) and (22) and are shown in column 6 of Table 1. Small disagreements here may be due to errors in the numerical solution.

In figure 1, the variation of s-wave phase shift $\delta_0$ with $k^2$ (energy) is shown for different values of the coupling constant "g" ranging from $g= 0.991 - 0.9935$. The variation in the values of $\delta_0$ is found to follow the same pattern. It is interesting to note that increases with an increase of $k^2$. This behaviour is in agreement with the result for non-relativistic particles obtained by Gammel et al. [19], Bransden [20] and Raghuwanshi [21]. As we keep on increasing the value of the coupling constant “g”, we found that s-wave phase shift $\delta_0$ increases for the same value of $k^2$.

REFERENCES


