On the Scattering Theory of the Dirac Equation*

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It is shown that for sufficiently strong potentials, the Born approximation is not valid even at very high energies. A variational principle is derived for the phase shifts and applied to a simple case. Two exact expressions for the phase shifts are also found.

I. INTRODUCTION

In the course of an investigation on the problem of the scattering of high energy electrons from heavy nuclei, a number of results in the scattering theory of the Dirac equation were obtained. In the following paragraph, the limitations of the Born approximation in the Dirac theory are investigated. It is shown that for sufficiently strong potentials the Born approximation is not valid at very high energies. This is done by interpreting the Born approximation in terms of the phase shifts and then investigating the behavior of the phase shifts at high energies.

A variational principle is derived for the phase shifts. A simple application of the variational principle gives a result for the phase shift which is more accurate than the Born approximation. In addition, two exact expressions for the phase shifts are found.

II. DEFINITION OF THE PHASE SHIFTS

The phase shift method was first applied to the Dirac equation by Mott[1] in calculating the Coulomb scattering of fast electrons. We shall write the Dirac equation for an electron moving in an electric field only as[2]

$$(H+V)\psi=E\psi,\quad H=-(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta). \tag{1}$$

In (1) we have used relativistic units, $\hbar=m=1=c$.

As with the non-relativistic Schroedinger equation, we can decompose the wave function into spherical harmonics.[3] Let us denote the radial parts of the wave function by $f_l(r)/r$ and $g_l(r)/r$; these functions satisfy the differential equations,

$$(d/dr)f_l=-(l+1/r)f_l+(E-V-1)g_l, \tag{2-a}$$

$$(d/dr)g_l=-(E-V+1)f_l+(l+1/r)g_l. \tag{2-b}$$

If $V(r)$, the potential, goes to zero faster than $1/r$ at ∞, then the functions g_l and f_l have the asymptotic forms,

$$g_l\rightarrow(E+1)^{\frac{1}{2}}\cos[kr-\tfrac{1}{2}(l+1)\pi+\delta_l], \tag{3-a}$$

$$f_l\rightarrow(E-1)^{\frac{1}{2}}\sin[kr-\tfrac{1}{2}(l+1)\pi+\delta_l]. \tag{3-b}$$

The δ_l defined by Eqs. (3) are the phase shifts; they are zero if $V(r)\equiv 0$. If the potential goes like ze^2/r at infinity, then there is the additional logarithmic term just as in the Schroedinger theory.

In terms of these phase shifts, one can write down the cross section for an unpolarized incoming beam of electrons as[1]

$$\sigma(\theta)=|f_3(\theta)|^2+|f_4(\theta)|^2, \tag{4}$$

where

$$f_3(\theta)=\frac{1}{k}\sum_{l=1}\left\{(l+1)\left[\frac{e^{2i\delta_l}-1}{2i}\right]+l\left[\frac{e^{2i\delta_{-l-1}}-1}{2i}\right]\right\}P_l(\cos\theta) \tag{5}$$

and

$$f_4(\theta)=\frac{1}{k}\sum_{l=0}\left\{\frac{e^{2i\delta_{-l-1}}-e^{2i\delta_l}}{2i}\right\}P_l^1(\cos\theta). \tag{6}$$

Here

$$P_l^1=\sin\theta dP_l(\cos\theta)/d(\cos\theta),$$

and the δ_{-l-1} are also defined by Eqs. (2) and (3), where l is replaced by $-l-1$.

In the non-relativistic limit, $\delta_l=\delta_{-l-1}$, so that in (5) and (6), $f_3(\theta)$ becomes the usual Schroedinger scattering amplitude,

$$f_3(\theta)=\frac{1}{k}\sum_{l=1}(2l+1)\left[\frac{e^{2i\delta_l}-1}{2i}\right]P_l(\cos\theta),$$

and $f_4(\theta)\equiv 0$.

III. THE VALIDITY OF THE BORN APPROXIMATION IN THE DIRAC THEORY

It has already been noted that the Born approximation does not give good results in the Coulomb scattering from heavy elements, even at very high energies.[4,5] We shall show that this is a general property of the Dirac equation; if the potential is sufficiently strong,[6] then no matter how high the energy of the scattered particle, the Born approximation will not be valid. This

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[1] N. F. Mott, Proc. Roy. Soc. **A 124**, 426 (1949).

[2] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 311.

[3] C. G. Darwin, Proc. Roy. Soc. **A 118**, 654 (1928).

[4] Bartlett and Watson, Proc. Am. Acad. **74**, 53 (1940).

[5] W. McKinley and H. Feshbach, Phys. Rev. **74**, 1759 (1948).

[6] A criterion for "sufficiently strong" is given later.

is in contrast to the Schroedinger equation, where the Born approximation will always be valid if we take the energy of the incident particle large enough.

To investigate the validity of the Born approximation we shall first express it in terms of conditions on the phase shifts. In the non-relativistic theory one can show that the Born approximation is equivalent to the assumption that the phase shifts are given by,

$$(e^{2i\delta_l}-1)/2i=-k\int_0^\infty 2\cdot V(r)\cdot j_l^2(kr)\cdot r^2\cdot dr, \qquad (7)$$

where $j_l(kr)$ is the spherical Bessel function.[7] We shall find a similar expression in the Dirac theory.

The Born approximation has been treated by others,[8] but we shall derive a somewhat different form of it which will be more useful for later work. Let us rewrite (1) as

$$(E+\boldsymbol{\alpha}\cdot\mathbf{p}+\beta)\psi=V\psi$$

and operate on both sides of the equation by

$$(E-\boldsymbol{\alpha}\cdot\mathbf{p}-\beta);$$

then because of the properties of the Dirac matrices we get

$$(\nabla^2+k^2)\psi=(E-\boldsymbol{\alpha}\cdot\mathbf{p}-\beta)\cdot V\psi, \qquad (8)$$

where $k=(E^2-1)^{\frac{1}{2}}$ is the momentum. Now let us suppose we have an incoming plane wave represented by $a_{\mathbf{k}_0}\exp(i\mathbf{k}_0\cdot\mathbf{r})$, where $a_{\mathbf{k}_0}$ is a spinor. The plane wave has a momentum $\mathbf{k}_0$ and energy $E=(k^2+1)^{\frac{1}{2}}$. The solution of (8) is obtained by the usual procedure of using the Green's function

$$-\frac{1}{4\pi}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}. \qquad (9)$$

The solution of (2), giving the scattering due to the potential $V(\mathbf{r})$, is then

$$\psi=a_{\mathbf{k}_0}e^{i\mathbf{k}_0\cdot\mathbf{r}}-\int\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\cdot[E-\boldsymbol{\alpha}\cdot\mathbf{p}'-\beta]\cdot V(\mathbf{r}')\cdot\psi(\mathbf{r}')\cdot d\mathbf{r}', \qquad (10)$$

where $\mathbf{p}$ is the operator, $-i$ grad. We can bring the operator $(E-\boldsymbol{\alpha}\cdot\mathbf{p}'-\beta)$ outside the integral sign by first integrating by parts and then noting that

$$\frac{\partial}{\partial x'}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}=-\frac{\partial}{\partial x}\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}. \qquad (11)$$

Thus we get,

$$\psi=a_{\mathbf{k}_0}e^{i\mathbf{k}_0\cdot\mathbf{r}}-[E-\boldsymbol{\alpha}\cdot\mathbf{p}-\beta]\int\frac{e^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi|\mathbf{r}-\mathbf{r}'|}\cdot V(\mathbf{r}')\cdot\psi(\mathbf{r}')\cdot d\mathbf{r}'. \qquad (12)$$

The asymptotic form of (12), which will yield the scattering amplitude, is

$$\psi\to a_{\mathbf{k}_0}e^{i\mathbf{k}\cdot\mathbf{r}_0}+\frac{e^{ikr}}{r}\cdot f(\theta,\varphi), \qquad (13)$$

and

$$f(\theta,\varphi)=-\frac{1}{4\pi}(E-\beta-\boldsymbol{\alpha}\cdot\mathbf{k})\cdot\int e^{-i\mathbf{k}\cdot\mathbf{r}}\cdot V(\mathbf{r})\cdot\psi(\mathbf{r})\cdot d\mathbf{r}, \qquad (14)$$

where $\mathbf{k}$ is the momentum vector in the direction θ, φ relative to the direction of $\mathbf{k}_0$. Here, of course, $f(\theta,\varphi)$ represents four functions, $f_i(\theta,\varphi)$, $i=1, 2, 3, 4$.

Equation (14) is a general expression for the scattering amplitude. To obtain the Born approximation from it, we replace $\psi(\mathbf{r})$ by its zero-order approximation $a_{\mathbf{k}_0}e^{i\mathbf{k}_0\cdot\mathbf{r}}$; thus in the Born approximation,

$$f(\theta,\varphi)=\tfrac{1}{2}(E-\beta-\boldsymbol{\alpha}\cdot\mathbf{k})\cdot a_{\mathbf{k}_0}\cdot f_{\text{n.r.}}(\theta,\varphi), \qquad (15)$$

where

$$f_{\text{n.r.}}(\theta,\varphi)=\frac{-2}{4\pi}\cdot\int e^{-i\mathbf{k}\cdot\mathbf{r}}\cdot V(\mathbf{r})\cdot e^{i\mathbf{k}_0\cdot\mathbf{r}}\cdot d\mathbf{r} \qquad (16)$$

and is the usual Born approximation for the non-relativistic Schroedinger equation.

From (15), we can obtain the differential cross section,

$$\sigma(\theta,\varphi)=|f(\theta,\varphi)|^2=\textstyle\sum_i|f_i(\theta,\varphi)|^2,$$

to check this expression for the scattering amplitude. Thus

$$\sigma=\tfrac{1}{4}\cdot a_{\mathbf{k}_0}^*\cdot[E-\beta-\boldsymbol{\alpha}\cdot\mathbf{k}]^2\cdot a_{\mathbf{k}_0}\cdot|f_{\text{n.r.}}|^2. \qquad (17)$$

Now

$$[E-\beta-\boldsymbol{\alpha}\cdot\mathbf{k}]^2=2E\cdot(E-\beta-\boldsymbol{\alpha}\cdot\mathbf{k}) \qquad (18)$$

since $\beta^2=1$, $\beta\boldsymbol{\alpha}+\boldsymbol{\alpha}\beta=0$ and $(\boldsymbol{\alpha}\cdot\mathbf{k})^2=k^2$. Thus

$$a_{\mathbf{k}_0}^*[E-\beta-\boldsymbol{\alpha}\cdot\mathbf{k}]^2a_{\mathbf{k}_0}=2E[E+(1/E)+\mathbf{v}_0\cdot\mathbf{k}]; \qquad (19)$$

since $a_{\mathbf{k}_0}^*\beta a_{\mathbf{k}_0}=-1/E$, and $a_{\mathbf{k}_0}^*\boldsymbol{\alpha}a_{\mathbf{k}_0}=-\mathbf{v}_0$, the initial velocity of the particle. Writing $vk\cos\theta$ for $\mathbf{v}_0\cdot\mathbf{k}$ in (19) and substituting into (17) we get for the cross section[9]

$$\sigma(\theta,\varphi)=\frac{1}{1-v_0^2}(1-v_0^2\sin^2\tfrac{1}{2}\theta)\cdot|f_{\text{n.r.}}|^2. \qquad (20)$$

Returning now to expression (15) for the scattering amplitude $f(\theta,\varphi)$; we wish to derive an expression for the phase shifts from it. This we will do by comparison of Eq. (15) with the expression for $f(\theta)$ in terms of the phase shifts; namely, Eqs. (5) and (6).

In Eq. (14), let us introduce the explicit forms for the matrices $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $a_{\mathbf{k}_0}$,

$$\boldsymbol{\alpha}=\begin{bmatrix}0 & \boldsymbol{\sigma}\\ \boldsymbol{\sigma} & 0\end{bmatrix},\quad \beta=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},$$
$$\sigma_x=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad \sigma_y=\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix},\quad \sigma_z=\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \qquad (21)$$

[7] Reference 2, p. 77.

[8] T. Sexl, Zeits. f. Physik **81**, 178 (1933).

[9] A similar result was obtained by time perturbation by M. E. Rose, Phys. Rev. **73**, 279 (1948).

and

$$a_{\mathbf{k}_0}=\begin{bmatrix}-k/(E+1)\\0\\1\\0\end{bmatrix}.$$

We have assumed the plane wave moving in the $+z$ direction and polarized with spin in the $+z$ direction. Then Eq. (15) gives for $f_3(\theta)$ and $f_4(\theta)$,

$$f_3(\theta)=\tfrac{1}{2}(E+1)\{1+(k/(E+1))^2\cos\theta\}\cdot f_{\mathrm{n.r.}}(\theta), \tag{22-a}$$

$$f_4(\theta)=\tfrac{1}{2}(E+1)\cdot(k/(E+1))^2\sin\theta\cdot f_{\mathrm{n.r.}}(\theta). \tag{22-b}$$

One may note that (22) has the correct non-relativistic limit. In this limit, $k\rightarrow 0$ to order v/c, $E\rightarrow 1$ to order $(v/c)^2$ and thus $f_3(\theta)\rightarrow f_{\mathrm{n.r.}}(\theta)$ and $f_4\rightarrow 0$ to order $(v/c)^2$.

Now compare expressions (22-a) and (5) for $f_3(\theta)$. Using the orthogonal property of Legendre polynomials, we get

$$(l+1)\frac{e^{2i\delta_l}-1}{2i}+l\frac{e^{2i\delta_{-l-1}}-1}{2i}=k\cdot\frac{2l+1}{2}\cdot\frac{E+1}{2}\cdot\int_0^\pi\left\{1+\left(\frac{k}{E+1}\right)^2\cos\theta\right\}\cdot f_{\mathrm{n.r.}}(\theta)\cdot P_l(\cos\theta)\sin\theta d\theta. \tag{23}$$

Now the expansion for $f_{\mathrm{n.r.}}(\theta)$ in terms of $P_l(\cos\theta)$ is given by the Schroedinger theory as

$$f_{\mathrm{n.r.}}(\theta)=\frac{1}{k}\sum_{l=0}(2l+1)\cdot\Delta_l\cdot P_l(\cos\theta), \tag{24}$$

where

$$\Delta_l=-k\int_0^\infty 2\cdot V(r)\cdot j_l^2(kr)\cdot r^2dr. \tag{25}$$

Δ_l is, as noted above, the non-relativistic Born approximation for $(e^{2i\delta_l}-1)/2i$.

Substituting (24) into (23), and using the relation

$$\int_{-1}^1 P_{l'}(x)\cdot P_l(x)\cdot x\cdot dx=\begin{cases}2(l+1)/(2l+1)(2l+3), & l'=l+1\\ 0, & l'\neq l\pm 1\\ 2l/(2l-1)(2l+1), & l'=l-1,\end{cases} \tag{26}$$

we get

$$\frac{l+1}{2l+1}\frac{e^{2i\delta_l}-1}{2i}+\frac{l}{2l+1}\frac{e^{2i\delta_{-l-1}}-1}{2i}=\frac{E+1}{2}\left\{\Delta_l+\left(\frac{k}{E+1}\right)^2\left[\frac{l}{2l+1}\Delta_l+\frac{l+1}{2l+1}\cdot\Delta_{l+1}\right]\right\}. \tag{27}$$

Equation (27) is one relation for δ_l and δ_{-l-1}; a second such relation will be obtained by treating $f_4(\theta)$ in a similar manner. As the functions $P_l'(\cos\theta)$ form an orthogonal set,

$$\int_{-1}^1 P_l{}^1\cdot P_{l'}{}^1\cdot dx=\delta_{ll'}\cdot\frac{2}{2l+1}\cdot l(l+1),$$

Eqs. (22-b) and (6) give,

$$\frac{e^{2i\delta_{-l-1}}-e^{2i\delta_l}}{2i}=\frac{k}{l(l+1)}\cdot\frac{2l+1}{2}\cdot\frac{E+1}{2}\cdot\left(\frac{k}{E+1}\right)^2\times\int_0^\pi\sin\theta\cdot f_{\mathrm{n.r.}}(\theta)\cdot P_l(\cos\theta)d(\cos\theta). \tag{28}$$

Again, substituting (24) for $f_{\mathrm{n.r.}}(\theta)$ and now using the integral,

$$\int_{-1}^1(1-x^2)^{\frac{1}{2}}\cdot P_{l'}{}^1(x)\cdot P_l{}^1(x)=\begin{cases}2l(l+1)/(2l+1)(2l-1), & l'=l-1\\ -2l(l+1)/(2l+1)(2l+3), & l'=l+1\\ 0, & l'\neq l\pm 1.\end{cases} \tag{29}$$

we get

$$\frac{e^{2i\delta_{-l-1}}-e^{2i\delta_l}}{2i}=\frac{E+1}{2}\cdot\left(\frac{k}{E+1}\right)^2\cdot\{\Delta_{l+1}-\Delta_l\}. \tag{30}$$

Equations (27) and (30) can be solved simultaneously for δ_l and δ_{-l-1}; thus,

$$(e^{2i\delta_l}-1)/2i=\tfrac{1}{2}(E+1)\{\Delta_l+(k/(E+1))^2\Delta_{l+1}\}, \tag{31-a}$$

$$(e^{2i\delta_{-l-1}}-1)/2i=\tfrac{1}{2}(E+1)\{\Delta_l+(k/(E+1))^2\Delta_{l-1}\}. \tag{31-b}$$

Use of the Born approximation in the Dirac theory is equivalent to calculating the phase shifts by means of Eqs. (31). In the non-relativistic limit, $E\rightarrow 1$, and we get $\delta_{-l-1}=\delta_l$ and $(e^{2i\delta_l}-1)/2i=\Delta_l$ as in the Schroedinger theory.

However, in the high energy limit, we get a result quite different from that expected in the Schroedinger theory. The phase shifts do not approach zero. If we assume the potential not to have a pole at $r=0$, then in Δ_l we can replace $j_l(kr)$ by its asymptotic form, $\sin(kr-\frac{1}{2}l\pi)/kr$. Equations (31) and (7) give,

$$\frac{e^{2i\delta_l}-1}{2i}\underset{k\rightarrow\infty}{\longrightarrow}-\int_0^\infty V(r)\cdot dr. \tag{32}$$

That is to say, for a given fixed energy, no matter how high, then for increasing l the phase shifts, of course, approach zero. But if we hold l fixed, then with increasing energy, the phase shift approaches a definite constant, independent of l, given by (32).

Let us call the phase shift at infinite energy δ_∞. We will show in the next section, that if the potential $V(r)$

has no pole at $r=0$, then δ_∞ is actually given by

$$\delta_\infty = -\int_0^\infty V(r)\cdot dr \tag{33}$$

and not only in the Born approximation.

Now (32) agrees with (33) to first order in V, as the Born approximation should. However if $\int_0^\infty V\cdot dr$ is large, then the Born approximation can be considerably in error. A criterion for the validity of the Born approximation is then (in ordinary c.g.s. units),

$$|\delta_\infty| = \left|(1/\hbar c)\cdot\int_0^\infty V(r)\cdot dr\right| \ll 1. \tag{34}$$

As a practical example, consider a square well based on the mercury nucleus. Let the range of the well be the radius a of the nucleus, and its depth be given by Ze^2/a. Then for this wall, $\delta_\infty=0.6$, which is not small. However for a square well based on hydrogen, δ_∞ would be small and the Born approximation would be valid for such a well.

The difference in the behavior of the Born approximation in the Dirac and Schroedinger theories can be understood qualitatively in the following manner. The Born approximation gives good results if the potential is weak, that is, if the wave function of the scattered particle is almost that of a free particle. Now in the Schroedinger theory, as we increase the energy of the particle, the potential becomes effectively weaker, since the particle spends less time near the scatterer. Thus, even for strong potentials, we can find energies high enough that the potential is effectively weak. However in the relativistic Dirac theory, this is not the case. For if the energy is already such that the particle is moving with almost the speed of light, increasing the energy now will not appreciably shorten the time spent by the particle in the neighborhood of the scatterer. Thus, if the Born approximation is not valid at energies of, for example, 10 mc^2, it will not be valid at any higher energies.

The above argument should hold for any relativistic equation. The phase shifts for the Klein-Gordon equation also exhibit the same properties as the Dirac phase shifts at high energies, indicating the non-validity of the Born approximation for sufficiently strong potentials in the case of the Klein-Gordon equation.

IV. THE PHASE SHIFTS AT INFINITE ENERGIES

In this section we deal with the behavior of the phase shifts at high energies and establish the result used in the previous section. It is convenient to introduce here a transformation used by Gordon[10] in finding the energy levels of the hydrogen atom.

Let $S_l(r)$ and $\bar{S}_l(r)$ be defined by

$$g_l = \tfrac{1}{2}(E+1)^{\frac{1}{2}}(S_l+\bar{S}_l), \tag{35-a}$$

and

$$f_l = -i\tfrac{1}{2}(E-1)^{\frac{1}{2}}(S_l-\bar{S}_l). \tag{35-b}$$

where $\bar{S}_l$ is the conjugate of S_l. $S_l(r)$ then has the asymptotic form, because of Eqs. (3),

$$S_l(r) \underset{r\to\infty}{\longrightarrow} e^{i(kr-\frac{1}{2}(l+1)\pi+\delta_l)}. \tag{36}$$

Also, by substituting (35) in Eqs. (2) for g_l and f_l we can obtain the differential equations for S_l,

$$\frac{d}{dr}S_l = \left(ik - i\frac{V}{k}\cdot E\right)S_l + \left(\frac{l+1}{r} - \frac{iV}{k}\right)\bar{S}_l, \tag{37-a}$$

$$\frac{d}{dr}\bar{S}_l = \left(-ik + i\frac{V}{k}\cdot E\right)\bar{S}_l + \left(\frac{l+1}{r} + \frac{iV}{k}\right)S_l. \tag{37-b}$$

As both $f_l=g_l=0$ at $r=0$, $S_l=\bar{S}_l=0$ at $r=0$.

For purposes of later comparison between the Dirac and Schroedinger equations, we now show that the Schroedinger equation can be put in a form almost identical with that of Eqs. (37).

For the moment, let $g_l(r)/r$ denote the radial part of the wave function in the Schroedinger theory; then $g_l(r)$ satisfies the equation

$$\frac{d^2}{dr^2}g_l + \left\{k^2 - 2\cdot V(r) - \frac{l(l+1)}{r^2}\right\}g_l = 0. \tag{38}$$

In order to proceed in a manner analogous to that in the Dirac theory, we rewrite (38) as two first-order equations. We introduce a function $f_l(r)$ defined by

$$-kf_l(r) = \frac{d}{dr}g_l - \frac{l+1}{r}g_l. \tag{39}$$

If the singularity of $V(r)$ at $r=0$ is not stronger than $1/r$, then $f_l=0$ at $r=0$. Equation (38) becomes now

$$\frac{d}{dr}f_l = \left(k - \frac{2V}{k}\right)g_l - \frac{l+1}{r}f_l. \tag{40}$$

Equations (39) and (40) are two first-order equations involving two functions, and are equivalent to Eq. (38).

Again we introduce the complex function $S_l(r)$, now defined by

$$g_l = \tfrac{1}{2}(S_l+\bar{S}_l), \tag{41-a}$$

$$f_l = -i\tfrac{1}{2}(S_l-\bar{S}_l). \tag{41-b}$$

$S_l(r)$ has the asymptotic form

$$S_l \to \exp[i(kr-\tfrac{1}{2}(l+1)\pi+\delta_l)]$$

and can be shown to obey the equation,

$$\frac{d}{dr}S_l = \left(ik - \frac{iV}{k}\right)S_l + \left(\frac{l+1}{r} - i\frac{V}{k}\right)\bar{S}_l, \tag{42-a}$$

$$\frac{d}{dr}\bar{S}_l = \left(-ik + \frac{iV}{k}\right)\bar{S}_l + \left(\frac{l+1}{r} + \frac{iV}{k}\right)S_l. \tag{42-b}$$

Also, as $f_l=g_l=0$ at $r=0$, the $S_l=\bar{S}_l=0$ at $r=0$.

[10] W. Gordon, Zeits. f. Physik **48**, 11 (1928).

It will be noted that Eqs. (37) in the Dirac theory become identical with Eqs. (42) in the Schroedinger theory if we put $E=1$ in (37). Equations (37) and (42) then make very clear the connection between the Dirac and Schroedinger equations. Also, any results we obtain in the Dirac theory using Eqs. (37) will likewise hold in the Schroedinger theory if we put $E=1$.

Returning now to the problem of calculating δ_∞, in Eq. (35), let

$$S_l(e)=e^{i\varphi(r)}S_l^0(r), \tag{43}$$

where $S_l^0(r)$ is the free particle wave function, a solution of (37) with $V\equiv 0$. Thus asymptotically, as $r\rightarrow\infty$, $\varphi(r)\rightarrow\delta_l$. Also, if $V(r)$ has no pole at $r=0$, S_l/S_l^0 is regular at $r=0$, so that $\varphi(r)$ and $d\varphi/dr$ are also regular at $r=0$.

By substituting (43) in (37), $\varphi(r)$ satisfies the equation,

$$\frac{d}{dr}\varphi=-\frac{V}{k}E+i\frac{l+1}{r}(\bar{S}_l^0/S_l^0)[1-e^{-i(\varphi+\bar{\varphi})}]-\frac{V}{k}(\bar{S}_l^0/S_l^0)e^{-i(\varphi+\bar{\varphi})}, \tag{44}$$

where $\bar{\varphi}$ is the complex conjugate φ.

Now if we assume $V(r)$ has no pole at $r=0$, then since $d\varphi/dr$ is regular at $r=0$, the $(l+1)/r$ term must be canceled. Thus we must have

$$\varphi+\bar{\varphi}=2Re(\varphi)=0,\ \text{at}\ r=0. \tag{45}$$

Take the conjugate of (44) and add it to (42); this gives after integration,

$$\tfrac{1}{2}(\varphi+\bar{\varphi})\Big]_0^\infty=-\int_0^\infty\frac{V}{k}\cdot E\cdot dr+\left\{\frac{i}{2}\int_0^\infty\frac{l+1}{r}[1-e^{-i(\varphi+\bar{\varphi})}]\frac{\bar{S}_l^0}{S_l^0}dr+\mathrm{cc}\right\}+\left\{-\int_0^\infty\frac{V}{2k}\frac{\bar{S}_l^0}{S_l^0}e^{-i(\varphi+\bar{\varphi})}\cdot dr+\mathrm{cc}\right\}. \tag{46}$$

Note that $\frac{1}{2}(\varphi+\bar{\varphi})]_0^\infty=\delta_l$, so that (46) is an expression for the phase shift. Now in the limit $k\rightarrow\infty$, the second integral $\rightarrow 0$ at least as fast as $1/k$. For let

$$\frac{l+1}{r}[1-e^{-i(\varphi+\bar{\varphi})}]=h(r). \tag{47}$$

$h(r)$ has no pole at $r=0$. When $r\rightarrow\infty$, $\varphi+\bar{\varphi}\rightarrow$ a constant and $h(r)\rightarrow\text{const.}/r$. So $h(r)$ is a smooth function. On the other hand $\bar{S}_l^0/S_l^0\rightarrow e^{-2ikr}$ for large k and r, and oscillates rapidly. Thus the integral $\int_0^\infty h(r)\cdot\bar{S}_l^0/S_l^0\cdot dr\rightarrow 0$ as least as fast as $1/k$ for high k.

Similarly the third integral in (46) $\rightarrow 0$ like $1/k^2$ for high k.

Thus,

$$\delta_l=-\int_0^\infty (V/k)\cdot Edr+O(1/k) \tag{48}$$

or

$$\delta_\infty=-(1/\hbar c)\int_0^\infty V(r)\cdot dr \tag{49}$$

(in ordinary c.g.s. units).

V. A VARIATIONAL PRINCIPLE FOR THE PHASE SHIFTS

In this section we derive a variational principle for the phase shifts. Let the integral I be defined by,

$$I=\frac{1}{2i}\int_0^\infty\left\{S_l\frac{d}{dr}\bar{S}_l-\bar{S}_l\frac{d}{dr}S_l+2iS_l\bar{S}_l\left(k-\frac{V}{k}\cdot E\right)+\left(\frac{l+1}{r}-\frac{iV}{k}\right)\bar{S}_l^2-\left(\frac{l+1}{r}+\frac{iV}{k}\right)\cdot S_l^2\right\}\cdot dr, \tag{50}$$

and let

$$J=\int_0^\infty S_l\left\{\frac{d}{dr}\bar{S}_l-\left(-ik+\frac{iV}{k}E\right)\cdot\bar{S}_l-\left(\frac{l+1}{r}+\frac{iV}{k}\right)\cdot S_l\right\}\cdot dr. \tag{51}$$

Then we have

$$I=-i\tfrac{1}{2}(J-\bar{J}), \tag{52}$$

where $\bar{J}$ is the complex conjugate of J. From (52) we observe that the integral I is real and that $I=0$ for the true wave function. Let us now introduce the trial junction $S_t(r)$ in I and J with the restrictions,

$$S_t(r)=0,\ \text{at}\ r=0,$$

$$S_t(r)\underset{r\rightarrow\infty}{\longrightarrow}\exp[i(kr+\eta_t)]=\exp i[kr-\tfrac{1}{2}(l+1)\pi+\delta_t], \tag{53}$$

$$\eta_t=\delta_t-\tfrac{1}{2}(l+1)\pi.$$

Forming the first variation of J, we get after integrating by parts

$$\delta J_t=S_t\cdot\delta\bar{S}_t\Big]_0^\infty+\int_0^\infty\left\{-\frac{dS_t}{dr}\cdot\delta\bar{S}_t-\left(-ik+\frac{iV}{k}\cdot E\right)\cdot S_t\cdot\delta\bar{S}_t-\left(\frac{l+1}{r}-\frac{iV}{k}\right)S_t\cdot\delta S_t\right\}\cdot dr. \tag{54}$$

But at infinity, $\delta\bar{S}_t=-i\delta\eta_t\exp(-ikr)$ and making use of Eq. (37) for S, Eq. (54) becomes

$$\delta J_t=-i\delta\eta_t-\tfrac{1}{2}\delta\cdot\int_0^\infty\left\{\left(\frac{l+1}{r}+\frac{iV}{k}\right)\bar{S}_t^2+\left(\frac{l+1}{r}-\frac{iV}{k}\right)S_t^2\right\}\cdot dr. \tag{55}$$

The last part is real and drops out in calculating δI_t which is the imaginary part of δJ_t. Thus we get our variational principle,

$$\delta\cdot\{I_t+\eta_t\}=0. \quad (56)$$

That is, if δ_l is the true phase shift, then as $I=0$ for the true wave function,

$$\delta_l=\text{extremum of }\{I_t+\delta_t\}. \quad (57)$$

Thus for any trial function S_t, obeying restrictions (53), we can calculate I_t and write, to first order,

$$\delta_l\cong I_t+\delta_t. \quad (58)$$

We might also point out that by simply putting $E=1$ in (50) and (56) we obtain a variational principle for the non-relativistic phase shift, where S is now the non-relativistic function defined in Section IV.

The simplest trial function to use in the solution $S_t(r)$ for some potential $V_t(r)$ and with the known phase shift δ_t. Putting $S_t(r)$ into (50) and (56) and using Eq. (37) for $S_t(r)$, obtain

$$\delta_l-\delta_t=-\frac{E}{k}\int_0^\infty (V-V_t)\times\left\{S_t\bar{S}_t+\frac{1}{2E}(S_t^2+\bar{S}_t^2)\right\}\cdot dr. \quad (59)$$

If we reintroduce the functions f_t and g_t, according to Eq. (41), then we can write (59) as

$$\delta_l-\delta_t=-\frac{E+1}{2k}\int_0^\infty 2\cdot(V-V_t)\cdot\left\{\frac{g_t^2}{E+1}+\left(\frac{k}{E+1}\right)^2\cdot\frac{f_t^2}{E-1}\right\}\cdot dr. \quad (60)$$

For the special case $V_t(r)\equiv 0$, $\delta_t=0$, the solutions for Eq. (2) can be shown to be,

$$g_l=(E+1)^{\frac{1}{2}}\cdot kr\cdot j_l(kr),\quad f_l=(E-1)^{\frac{1}{2}}\cdot kr\cdot j_{l+1}(kr),$$

and

$$g_{-l-1}=(E+1)^{\frac{1}{2}}\cdot kr\cdot j_l(kr),$$
$$f_{-l-1}=-(E-1)^{\frac{1}{2}}\cdot kr\cdot j_{l-1}(kr).$$

Thus,

$$\delta_l=\tfrac{1}{2}(E+1)\{\Delta_l+(k/(E+1))^2\Delta_{l+1}\}, \quad (61\text{-a})$$

$$\delta_{-l-1}=\tfrac{1}{2}(E+1)\{\Delta_l+(k/(E+1))^2\Delta_{l-1}\}. \quad (61\text{-b})$$

where the Δ_l are as defined in Section III,

$$\Delta_l=-k\int_0^\infty 2\cdot V(r)\cdot j_l^2(kr)\cdot r^2\cdot dr. \quad (62)$$

The variational result (61) is identical with the Born approximation except that $(e^{2i\delta_l}-1)/2i$ is replaced by δ_l. However (61) gives the correct limit for the phase shifts when $E\rightarrow\infty$, $\delta_\infty=-\int_0^\infty V\cdot dr$. Thus for a strong potential, where the phase shift may be large even at high energies, the variational results (60) and (61) are considerably better than the Born approximation.

As other writers[11] have already pointed out in connection with the Schroedinger theory, the variational principle for the phase shift provides neither an upper nor a lower bound. Thus it has the disadvantage that adding more parameters to the trial function does not necessarily give better results for the phase shift.

VI. SOME NUMERICAL RESULTS FOR THE PHASE SHIFTS OF A SQUARE WELL

In order to illustrate the behavior of the phase shifts in the Dirac theory, we shall do a numerical calculation for a square well of depth V_0 and range a. We shall calculate the phase shifts exactly and also by use of the variational formula (61), and compare the results.

For a constant potential $-V_0$, the solution of Eqs. (2) for f_l and g_l are

$$g_l=(E+V_0+1)^{\frac{1}{2}}\cdot kr\cdot j_l(pkr), \quad (63\text{-a})$$

and

$$f_l=(E+V_0-1)^{\frac{1}{2}}\cdot kr\cdot j_{l+1}(pkr), \quad (63\text{-b})$$

where

$$p=\left[1+2\cdot\frac{V_0}{k}\frac{E}{k}+\left(\frac{V_0}{k}\right)^2\right]^{\frac{1}{2}}.$$

By matching this solution at $r=a$ to the free particle solutions, we find the phase shift as

$$\tan\delta_l=\frac{((E+1)/(E-1))^{\frac{1}{2}}j_l(ka)-\gamma_l j_{l+1}(ka)}{((E+1)/(E-1))^{\frac{1}{2}}n_l(ka)-\gamma_l\cdot n_{l+1}(ka)}, \quad (64)$$

where

$$\gamma_l=g_l/f_l|_{ka}=\left(\frac{E+V_0+1}{E+V_0-1}\right)^{\frac{1}{2}}\cdot\frac{j_l(pka)}{j_{l+1}(pka)}$$

and $n_l(kr)$ is the spherical Bessel function,

$$n_l(x)=(\pi/2x)^{\frac{1}{2}}\cdot(-1)^{l+1}\cdot J_{-l-\frac{1}{2}}(x).$$

The phase shift at infinite energy can be found directly from (64) by substituting the asymptotic forms of the Bessel functions. We get

$$\delta_\infty=V_0a$$

which agrees with our more general result.

For our numerical calculation, we put $V_0=21.8$ Mev, which is approximately the Coulomb potential at the center of a uniformly charged lead nucleus, and let $a=8.09\times10^{-13}$ cm which is about the radius of a lead nucleus. As our scattered particles we take 100-Mev electrons.

With these figures $\delta_\infty=0.9$ radian, a rather large phase shift. Table I lists the exact phase shifts and those calculated by the variational result, (61). δ_0 has

[11] L. Hulthén, Arkiv. f. Mat., Astr. o. Fys. **35A**, No. 25 (1948).

very nearly its asymptotic value of $\delta_\infty=0.9$. The phase shifts start out rather large, but decrease very rapidly with increasing l. The variational result gives good agreement for the first few δ_l and for the high δ_l. The agreement is worse for the intermediate δ_l.

TABLE I. Phase shifts for a 100-Mev electron scattered from a potential well, depth 21.8 Mev and range 8.09×10^{-13} cm, according to the Dirac equation. The exact phase shifts are compared with those obtained by the variational result (61).

l	Exact δ	δ by relation (61)
0	0.857	0.864
1	0.823	0.844
2	0.723	0.525
3	0.273	0.179
4	0.0471	0.0369
5	0.0055	0.0050
6	0.00054	0.00049

VII. TWO EXACT EXPRESSIONS FOR THE PHASE SHIFTS

We shall now derive two exact expressions for the phase shift. If we multiply both sides of Eq. (35-a) by $\exp[-i(kr-\frac{1}{2}(l+1)\pi)]$ and note that

$$e^{-ikr}\frac{d}{dr}S_l=\frac{d}{dr}(e^{-ikr}S_l)+ike^{-ikr}S_l \tag{65}$$

then by integrating and using the property $S_l=0$ at $r=0$ we get

$$e^{i\delta_l}=\int_0^\infty e^{-i[kr-\frac{1}{2}(l+1)\pi]}\times\left\{-\frac{iV}{k}\cdot E\cdot S_l+\left(\frac{l+1}{r}-\frac{iV}{k}\right)\bar{S}_l\right\}\cdot dr. \tag{66}$$

The expression (66) for the phase shift differs from usual expressions for the phase shift, and is simpler in that instead of involving the product of two wave functions one of the wave functions is replaced by what is essentially its asymptotic form, the elementary function $\exp[-i(kr-\frac{1}{2}(l+1)\pi)]$.

Relation (66) will also hold in the Schroedinger theory if we put $E=1$. It is simpler to discuss (66) in this non-relativistic limit. If we substitute for S_l in (66), the solutions for $V(r)\equiv0$, we get the approximate expressions for the phase shift,

$$\sin\delta_l\cong-k\int_0^\infty 2\cdot V(r)\cdot\frac{\cos[kr-\frac{1}{2}(l+1)\pi]}{kr}j_l(kr)\cdot r^2\cdot dr. \tag{67}$$

Equation (67) resembles the Born approximation for the phase shift: $(e^{2i\delta_l}-1)/2i$ is replaced by $\sin\delta_l$, which is not too important in the Schroedinger theory since δ_l is not large, and one of the spherical Bessel functions is replaced by its asymptotic form. Equation (67) does not give the phase shift correct to the first order in the potential, for then the term in the integrand of (66) involving $(l+1)/r$ would require that $\bar{S}_l(r)$ should be correct to first order in the potential. Also, one would not usually expect (67) to be better than the Born approximation as the asymptotic form of $j_l(kr)$ is a worse approximation to the true wave function near $r=0$ than is $j_l(kr)$.

However, the advantage of (66) would lie in using wave functions which are better approximations to the true wave function than are the free particle functions, and then making use of the simpler integrand to do the integration.

A second exact expression for the phase shift in the Dirac theory can be derived which is more analogous to the non-relativistic expression,

$$\sin\delta_l=-\int_0^\infty 2\cdot V(r)\cdot j_l(kr)\cdot g_l\cdot r\cdot dr.$$

Let us differentiate Eq. (2-b) and eliminate df_l/dr by means of (2-a); then we get the second-order equation for $g_l(r)$,

$$\frac{d^2}{dr^2}g_l+\left(k^2-\frac{l(l+1)}{r^2}\right)g_l=(2E-V)\cdot V\cdot g_l+\frac{dV}{dr}\cdot f_l. \tag{68}$$

Let $f_l^0(r)$ and $g_l^0(r)$ be the solutions of (2) for zero potential. By (68), $g_l^0(r)$ satisfies,

$$\frac{d^2}{dr^2}g_l^0+\left(k^2-\frac{l(l+1)}{r^2}\right)g_l^0=0. \tag{69}$$

Now multiply (68) by g_l^0, (69) by g_l, subtract and integrate. Then, using the asymptotic forms of g_l and g_l^0,

$$-(E+1)\cdot k\cdot\sin\delta_l=\int_0^\infty g_l^0(r)\left\{(2E-V)\cdot V\cdot g_l+\frac{dV}{dr}\cdot f_l\right\}\cdot dr. \tag{70}$$

If we now integrate the term involving dV/dr by parts, and eliminate df_l/dr and dg_l/dr by means of (2), we obtain finally

$$\sin\delta_l=-(1/2k)\int_0^\infty 2\cdot V(r)\cdot\{g_l^0g_l+f_l^0f_l\}\cdot dr. \tag{71}$$

Substituting the free particle wave functions given in Section VI, we get,

$$\sin\delta_l=-\tfrac{1}{2}(E+1)^{\frac{1}{2}}\int_0^\infty 2\cdot V(r)\cdot r\cdot\left\{j_l(kr)\cdot g_l(r)+\left(\frac{E-1}{E+1}\right)^{\frac{1}{2}}j_{l+1}(kr)\,f_l(r)\right\}\cdot dr, \tag{72-a}$$

$$\sin\delta_{-l-1} = -\tfrac{1}{2}(E+1)^{\frac{1}{2}} \int_0^\infty 2\cdot V(r)\cdot r\cdot \left\{ j_l(kr)\cdot g_l(r) - \left(\frac{E-1}{E+1}\right)^{\frac{1}{2}} j_{l-1}(kr)\cdot f_{-l-1}(r) \right\}\cdot dr. \quad \text{(72-b)}$$

The zeroth approximation to the wave functions will cause Eqs. (67) to yield a first-order approximation which will agree with the Born approximation in the Dirac theory except that $(e^{2i\delta_l}-1)/2i$ is replaced by $\sin\delta_l$.

A result similar to relation (66) will hold for potentials that go like Ze^2/r at infinity. We simply replaced in (66), the free particle solutions g_l^0 and f_l^0 by the Coulomb solutions and the potential $V(r)$ by the deviation from the pure Coulomb potential Ze^2/r.

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The Evaluation of the Collision Matrix

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Dyson's systematic approach to the reduction of the Heisenberg S-Matrix into a sum of "graph" terms can be simplified. A notation is introduced and an algebraic theorem is proved, which allow one to handle the reduction problem quite easily and in the same manner for any type of field.

I. INTRODUCTION

The Feynman technique[1] for calculating transition probabilities is now so widely used that a full and satisfactory understanding of it by a wider circle is desirable. An important step in this direction has been Dyson's[2] direct derivation of the method from a simple expression for the S-matrix. One feels, however, that the *pedagogical* value of Dyson's proof is slightly marred by certain omissions and obscurities; moreover, some of the algebraic considerations seem more involved than should be necessary. The purpose of this note is to supply a simple and straightforward proof. The case of the electron-positron field interacting with a quantized electromagnetic field is sufficiently general to allow us to demonstrate all of the features of the method.

Let then $\psi(x)$ be the Dirac field operator at the space-time point x, $\psi^\dagger$ the hermitian-conjugate of ψ, $\bar{\psi}=\psi^\dagger\beta$ the adjoint, and $A_\mu(x)$ the μ-th component of the electromagnetic potential. The S-matrix for the system can be written:

$$S = 1 + S_1 + S_2 + \cdots \quad (1)$$

where S_n, the term of the n-th order in the electron charge ϵ is expressed by a multiple integral over a product of field factors ψ, $\bar{\psi}$, A [Eq. (18) below]. Our problem is the reduction of S_n to a sum of terms *à la* Feynman. To this end we notice that our fields ψ and A are linear combinations of creation and destruction operators. For example, $\psi(x)=\sum_r a_r\psi_r(x)$ where the ψ_r's are the normalized representatives of the states of a free Dirac particle, and a_r is a destruction (creation) operator if r is a positive (negative) energy state. Collecting all the positive energy states together into a term $u(x)$ and the negative states into a term $\bar{v}(x)$ we can write:

$$\psi(x) = u(x) + \bar{v}(x), \quad \bar{\psi}(x) = \bar{u}(x) + v(x), \quad (2)$$

where u ($\bar{u}$) destroys (creates) electrons, and v ($\bar{v}$) destroys (creates) positrons.[3] Similarly, we can write

$$A_\mu(x) = a_\mu(x) + a_\mu^\dagger(x), \quad (2')$$

where $a_\mu(a_\mu^\dagger)$ destroys (creates) photons.[4] Substituting such expressions into a product of fields, we can expand each product into a sum of products in which each factor is either a creation or a destruction operator.

Following an idea of Houriet and Kind,[5] we then proceed to rearrange such a product so as to carry all creation operators to the left of all destruction operators, writing for instance: $u(x)\bar{v}(y) = -\bar{v}(y)u(x)$, $u(x)\bar{u}(y) = \{u(x), \bar{u}(y)\} - \bar{u}(y)u(x)$ where the anticommutator $\{u, \bar{u}\} = u\bar{u} + \bar{u}u$ is a c-number. Thus one may transform a product of n creation and destruction operators into the "ordered" product of the same factors, plus extra terms in which some pairs of factors have been replaced by their commutators or anticommutators while the remaining factors are "ordered" in the above sense. The advantage of this is that when we take the matrix element of an ordered product between a final and an

[1] R. P. Feynman, Phys. Rev. **76**, 749 (1949).
[2] F. J. Dyson, Phys. Rev. **75**, 486 (1949).

[3] We set $\bar{u}=u^\dagger\beta$, $v=\bar{v}^\dagger\beta$ or $\bar{v}=\beta v^\dagger$; the asymmetry in the definition of $\bar{u}$ and $\bar{v}$ shall not cause any trouble here.
[4] $a_\mu^\dagger$ is the hermitian conjugate of a_μ (of $-a_\mu$ if $\mu=4$). As regards the treatment of timelike photons, see Section IV.
[5] A. Houriet and A. Kind, Helv. Phys. Acta **22**, 319 (1949).