CALCULATION OF SCATTERING PHASE SHIFTS WITH INCLUSION OF THE SECOND APPROXIMATION

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The elastic scattering phase shifts for Dirac particles are determined from the interaction potential with inclusion of the second approximation. The results of the Born approximation and of damping theory, and also the McKinley-Feshbach formula, which is a generalization of the Rutherford-Mott formula, can be obtained as special cases.

1. INTRODUCTION

As is well known, in the theory of scattering one has the following exact formula for the angular distribution of a beam of unpolarized Dirac particles scattered by a stationary center of force:[1]

$$d\sigma / d\Omega = |f(\theta)|^2 + |g(\theta)|^2; \tag{1}$$

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}[(l+1)(\exp\{2i\delta_l^{(1)}\}-1) + l(\exp\{2i\delta_l^{(2)}\}-1)]P_l(\cos\theta),$$

$$g(\theta) = \frac{1}{2ik}\sum_{l=1}^{\infty}[-\exp\{2i\delta_l^{(1)}\}+\exp\{2i\delta_l^{(2)}\}]P_l^1(\cos\theta). \tag{2}$$

For the total effective cross-section we have:

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}[(l+1)\sin^2\delta_l^{(1)} + l\sin^2\delta_l^{(2)}]. \tag{3}$$

In the general case of an arbitrary interaction potential no exact expression has been found for the angles $\delta_l^{(1)}$ and $\delta_l^{(2)}$, which are the phase differences between the asymptotic expressions for the radial functions with the scattering center present and the radial functions of the free motion. There are various methods for the approximate calculation of the phase shifts $\delta_l^{(1)}$ and $\delta_l^{(2)}$, in particular the Born approximation and the semi-analytical method of Wentzel, Kramers, and Brillouin. Recently the phase shifts have been calculated by means of a damping theory.[2] In the present paper the phase shifts are calculated correct to the second approximation in the interaction potential. We note that if we confine ourselves to just the first approximation we shall get again the results of the damping theory.

2. SOLUTION OF THE DIRAC EQUATION FOR THE FREE PARTICLE

In studying the phase shifts for the elastic scattering of spinning particles it is convenient to take the solution of the free-particle Dirac equation

$$(E - c\mathbf{p}\cdot\boldsymbol{\alpha} - \rho_3 mc^2)\psi(\mathbf{r}) = 0, \tag{4}$$

without restriction by boundary conditions at infinity or at the origin, in the form:

$$\psi(\mathbf{r}) = \sum_l \begin{pmatrix} \sqrt{1+k_0/K}\{(l+1)A_l[j_l(kr) - \tan\delta_l^{(1)}n_l(kr)] \\ + lB_l[j_l(kr) - \tan\delta_l^{(2)}n_l(kr)]\}i^lP_l(\cos\theta) \\ \sqrt{1+k_0/K}\{A_l[j_l(kr) - \tan\delta_l^{(1)}n_l(kr)] \\ - B_l[j_l(kr) - \tan\delta_l^{(2)}n_l(kr)]\}i^le^{i\varphi}P_l^1(\cos\theta) \\ \sqrt{1-k_0/K}\{lA_{l-1}[j_l(kr) - \tan\delta_{l-1}^{(1)}n_l(kr)] \\ + (l+1)B_{l+1}[j_l(kr) - \tan\delta_{l+1}^{(2)}n_l(kr)]\}i^lP_l(\cos\theta) \\ \sqrt{1-k_0/K}\{-A_{l-1}[j_l(kr) - \tan\delta_{l-1}^{(1)}n_l(kr)] \\ + B_{l+1}[j_l(kr) - \tan\delta_{l+1}^{(2)}n_l(kr)]\}i^le^{i\varphi}P_l^1(\cos\theta) \end{pmatrix} \tag{5}$$

For $\delta_l^{(1)} = \delta_l^{(2)} = 0$ this solution describes a particle with positive energy and its momentum and spin directed along the z axis. Here

$$j_l(kr) = (\pi/2kr)^{1/2}J_{l+1/2}(kr); \quad n_l(kr) = (\pi/2kr)^{1/2}N_{l+1/2}(kr).$$

The quantity $\hbar k$ is the momentum, $E = c\hbar K$ is the energy, and $m = \hbar k_0/c$ is the mass of the particle. We note that, for $A_l = B_l = 1$ and $\delta_l^{(1)} = \delta_l^{(2)} = 0$, Eq. (5) is the expression of a plane wave in spherical coordinates.

The free-particle solution (5) is at the same time also an asymptotic expression for the solution of the Dirac equation in the presence of a spherically symmetrical center of short-range forces. In this case $\delta_l^{(1)}$ and $\delta_l^{(2)}$ are no longer arbitrary constants, and depend in a definite way on the form of the interaction potential.

3. APPROXIMATE SOLUTION OF THE DIRAC EQUATION FOR A PARTICLE IN A CENTRAL FIELD

In scattering problems the most important case is that in which there is no vector potential and the scalar potential is spherically symmetrical.

In this case it is convenient to consider instead of the Dirac equation

$$(E - c\,\mathbf{p}\cdot\boldsymbol{\alpha} - \rho_3 mc^2 - V(r))\,\psi(\mathbf{r}) = 0 \tag{6}$$

the equivalent integral equation

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \hat{D}(\mathbf{r})\int G(\mathbf{r},\mathbf{r}')V(r')\psi(\mathbf{r}')d\mathbf{r}', \tag{7}$$

where

$$G(\mathbf{r},\mathbf{r}') = -\frac{1}{4\pi}\frac{\cos k|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}'|}, \tag{8}$$

$$\hat{D}(\mathbf{r}) = c^{-2}\hbar^{-2}(E + c\mathbf{p}\cdot\boldsymbol{\alpha} + \rho_3 mc^2). \tag{9}$$

Furthermore for the zeroth approximation $\psi_0(\mathbf{r})$ we take not a plane wave, but the solution (5) of the free-particle Dirac equation, with the condition $\delta_l^{(1)} = \delta_l^{(2)} = 0$, which secures the finiteness of $\psi_0(\mathbf{r})$ at the origin:

$$\psi_0(\mathbf{r}) = \sum_l \begin{Bmatrix} \sqrt{\alpha}[(l+1)A_l + lB_l]\,i^l j_l(kr)P_l(\cos\theta) \\ \sqrt{\alpha}(A_l - B_l)i^l j_l(kr)\,e^{i\varphi}P_l^1(\cos\theta) \\ \sqrt{\beta}[lA_{l-1} + (l+1)B_{l+1}]i^l j_l(kr)\,P_l(\cos\theta) \\ \sqrt{\beta}(-A_{l-1} + B_{l+1})i^l j_l(kr)\,e^{i\varphi}P_l^1(\cos\theta) \end{Bmatrix} \tag{10}$$

where for convenience we have introduced the notations

$$\alpha = 1 + k_0/K, \qquad \beta = 1 - k_0/K.$$

Assuming that the interaction energy can be regarded as a perturbation, we carry out a successive-approximation calculation to the second order. In this approximation the wave function has the form:

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r}) + \psi_2(\mathbf{r})$$
$$= \psi_0(\mathbf{r}) + \hat{D}(\mathbf{r})\int G(\mathbf{r},\mathbf{r}')V(r')\psi_0(\mathbf{r}')d\mathbf{r}'$$
$$+ \hat{D}(\mathbf{r})\int G(\mathbf{r},\mathbf{r}')V(r')d\mathbf{r}'\,\hat{D}(\mathbf{r}')\int G(\mathbf{r}',\mathbf{r}'')V(r'')\psi_0(\mathbf{r}'')d\mathbf{r}''. \tag{11}$$

By using the arbitrariness of A_l and B_l, and also the choice of the Green's function (8), we try to identify the asymptotic form of the wave function with the conditions at infinity, Eq. (5), in first and second approximations. In what follows we use the following expansion of the Green's function:

$$-\frac{1}{4\pi}\frac{\cos k|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}'|}$$
$$= \frac{k}{4\pi}\sum_{l=0}^{\infty}(2l+1)G(r,r')\Big\{P_l(\cos\theta)P_l(\cos\theta')$$
$$+ 2\sum_{m=1}^{\infty}\frac{(l-m)!}{(l+m)!}P_l^m(\cos\theta)P_l^m(\cos\theta')\cos m(\varphi-\varphi')\Big\}, \tag{12}$$

$$G(r,r') = \begin{cases} j_l(kr')\,n_l(kr) & \text{for } r > r', \\ j_l(kr)\,n_l(kr') & \text{for } r < r'. \end{cases}$$

Here $\mathbf{r}$, θ, φ and $\mathbf{r}'$, θ', φ' respectively are the spherical coordinates for the position vectors $\mathbf{r}$ and $\mathbf{r}'$.

(a) First approximation. In the first approximation

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r})$$
$$= \psi_0(\mathbf{r}) + \hat{D}(\mathbf{r})\int G(\mathbf{r},\mathbf{r}')V(r')\psi_0(\mathbf{r}')d\mathbf{r}'. \tag{13}$$

By taking into account Eqs. (10), (12), and (13), and also the well known orthogonality and normalization relations of the Legendre polynomials, we can carry out the integration over the angles in $\psi_1(\mathbf{r})$. This gives:

$$\psi_1(\mathbf{r}) = k\hat{D}(\mathbf{r})\sum_l \begin{Bmatrix} \sqrt{\alpha}[(l+1)A_l + lB_l]i^l\Phi_l^l(r)P_l(\cos\theta) \\ \sqrt{\alpha}(A_l - B_l)i^l\Phi_l^l(r)e^{i\varphi}P_l^1(\cos\theta) \\ \sqrt{\beta}[lA_{l-1} + (l+1)B_{l+1}]i^l\Phi_l^l(r)P_l(\cos\theta) \\ \sqrt{\beta}(-A_{l-1} + B_{l+1})i^l\Phi_l^l(r)e^{i\varphi}P_l^1(\cos\theta) \end{Bmatrix} \tag{14}$$

where we have used the notation:

$$\Phi_l^m(r) = n_l(kr)\int_0^r j_m^2(kr')V(r')r'^2dr'$$
$$+ j_l(kr)\int_r^{\infty} n_m(kr')j_m(kr')V(r')r'^2dr'. \tag{15}$$

To get the final form of the wave function in first approximation, we must work out the application of the operator $\hat{D}(\mathbf{r})$ in the expression (14); we find as the result

$$\psi_1(\mathbf{r}) = \frac{kK}{c\hbar}\sum_l \begin{Bmatrix} \sqrt{\alpha}\{(l+1)A_l[\alpha\Phi_l^l(r) + \beta\Phi_l^{l+1}(r)] \\ + lB_l[\alpha\Phi_l^l(r) + \beta\Phi_l^{l-1}(r)]\}i^lP_l(\cos\theta) \\ \sqrt{\alpha}\{A_l[\alpha\Phi_l^l(r) + \beta\Phi_l^{l+1}(r)] - B_l[\alpha\Phi_l^l(r) \\ + \beta\Phi_l^{l-1}(r)]\}i^le^{i\varphi}P_l^1(\cos\theta) \\ \sqrt{\beta}(lA_{l-1}[\alpha\Phi_l^{l-1}(r) + \beta\Phi_l^l(r)] \\ + (l+1)B_{l+1}[\alpha\Phi_l^{l+1}(r) + \beta\Phi_l^l(r)]\}i^lP_l(\cos\theta) \\ \sqrt{\beta}\{-A_{l-1}[\alpha\Phi_l^{l-1} + \beta\Phi_l^l(r)] \\ + B_{l+1}[\alpha\Phi_l^{l+1}(r) + \beta\Phi_l^l(r)]\}i^le^{i\varphi}P_l^1(\cos\theta) \end{Bmatrix} \tag{16}$$

In obtaining Eq. (16) from Eq. (14) we have used the differential relations

$$(p_1 + ip_2)\,\Phi_l^l(r)\,P_l(\cos\theta)$$

$$= \frac{\hbar k e^{i\varphi}}{i(2l+1)}\,[\Phi_{l-1}^l(r)\,P_{l-1}^1(\cos\theta) + \Phi_{l+1}^l(r)P_{l+1}^1(\cos\theta)]$$

$$p_3\Phi_l^l(r)\,P_l(\cos\theta)$$

$$= \frac{\hbar k}{i(2l+1)}\,[l\Phi_{l-1}^l(r)\,P_{l-1}(\cos\theta) - (l+1)\Phi_{l+1}^l(r)P_{l+1}(\cos\theta)],$$

$$(p_1 - ip_2)\,\Phi_l^l(r)P_l^1(\cos\theta)e^{i\varphi}$$

$$= -\frac{\hbar k}{i}\,\frac{l(l+1)}{2l+1}\,[\Phi_{l-1}^l(r)P_{l-1}(\cos\theta)$$

$$+ \Phi_{l+1}^l(r)\,P_{l+1}(\cos\theta)],$$

$$p_3\Phi_l^l(r)P_l^1(\cos\theta)\,e^{i\varphi} = \frac{\hbar k e^{i\varphi}}{i(2l+1)}\,[(l+1)\Phi_{l-1}^l(r)\,P_{l-1}^1(\cos\theta)$$

$$- l\Phi_{l+1}^l(r)P_{l+1}^1(\cos\theta)], \qquad (17)$$

which can easily be obtained by direct differentiation if one uses the connections between the successive Legendre polynomials that are well known from the theory of spherical harmonics.

We note that in Eq. (16) only Legendre functions of order l appear; this formulation is obtained by replacements of the summation index l by $l-1$ and $l+1$.

Recalling the asymptotic behavior of the function $\Phi_l^m(r)$ for large r

$$\Phi_l^m(r) \to n_l(kr)\int_0^\infty j_m^2(kr')V(r')\,r'^2dr', \qquad (18)$$

and using Eqs. (10) and (16), we can easily write out the asymptotic expression for the first-approximation wave function $\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r})$. Identifying this with the expression (5), we determine the following values for the scattering phase shifts:

$$\tan\delta_l^{(1)} = -\frac{kK}{c\hbar}\left\{\alpha\int_0^\infty j_l^2(kr)\,V(r)\,r^2dr + \beta\int_0^\infty j_{l+1}^2(kr)\,V(r)\,r^2dr\right\},$$

$$\tan\delta_l^{(2)} = -\frac{kK}{c\hbar}\left\{\alpha\int_0^\infty j_l^2(kr)\,V(r)\,r^2dr + \beta\int_0^\infty j_{l-1}^2(kr)\,V(r)\,r^2dr\right\}. \qquad (19)$$

This same result is given also by the damping theory developed in the papers of reference 2. These papers contain a more detailed discussion of the results that follow from the formulas (19).

(b) Second approximation. The exact calculation of

$$\psi_2(\mathbf{r}) = \hat{D}(\mathbf{r})\int G(\mathbf{r},\mathbf{r}')\,V(r')\,\psi_1(\mathbf{r}')\,dr' \qquad (20)$$

involves rather cumbersome manipulations. We shall be interested in only the asymptotic behavior of $\psi(\mathbf{r}) = \psi_0(\mathbf{r}) + \psi_1(\mathbf{r}) + \psi_2(\mathbf{r})$, which is enough for the calculation of the scattering phase shifts in second approximation.

Substituting Eq. (16) in Eq. (20) and carrying out the angular integrations, we get by using Eq. (18) the asymptotic expression for $\psi_2(\mathbf{r})$ for $r \to \infty$:

$$\psi_2(\mathbf{r}) \approx \hat{D}(\mathbf{r})\sum_l \frac{Kk^2}{c\hbar}\begin{Bmatrix} \sqrt{\alpha}\,[(l+1)A_l\varepsilon_l^{(2)} \\ + lB_l\varepsilon_l^{(1)}]\,i^l n_l(kr)P_l(\cos\theta) \\ \sqrt{\alpha}[A_l\varepsilon_l^{(2)} - B_l\varepsilon_l^{(1)}]\;i^l n_l(kr)\,e^{i\varphi}P_l^1(\cos\theta) \\ \sqrt{\beta}[lA_{l-1}\varepsilon_l^{(4)} \\ + (l+1)B_{l+1}\varepsilon_l^{(3)}]\,i^l n_l(kr)P_l(\cos\theta) \\ \sqrt{\beta}[-A_{l-1}\varepsilon_l^{(4)} \\ + B_{l+1}\varepsilon_l^{(3)}]\;i^l n_l(kr)\,e^{i\varphi}P_l^1(\cos\theta), \end{Bmatrix} \qquad (21)$$

where

$$\varepsilon_l^{(1)} = \int_0^\infty j_l(kr')[\alpha\Phi_l^l(r') + \beta\Phi_l^{l-1}(r')]r'^2dr',$$

$$\varepsilon_l^{(2)} = \int_0^\infty j_l(kr')\,[\alpha\Phi_l^l(r') + \beta\Phi_l^{l+1}(r')]\,r'^2dr',$$

$$\varepsilon_l^{(3)} = \int_0^\infty j_l(kr')[\alpha\Phi_l^{l+1}(r') + \beta\Phi_l^l(r')]\,r'^2dr',$$

$$\varepsilon_l^{(4)} = \int_0^\infty j_l(kr')[\alpha\Phi_l^{l-1}(r') + \beta\Phi_l^l(r')]\,r'^2dr'. \qquad (22)$$

Equation (21) does not differ in its structure from Eq. (14), since the relations (17) also hold for the function $n_l(kr)$. Therefore we omit the computations and give the expressions for the phase shifts in second approximation:

$$\tan\delta_l^{(1)} = -\left(\frac{kK}{c\hbar}\right)\left\{\alpha\int_0^\infty j_l^2(kr)\,V(r)\,r^2dr + \beta\int_0^\infty j_{l+1}^2(kr)\,V(r)r^2dr\right\}$$

$$- \left(\frac{kK}{c\hbar}\right)^2\left\{\alpha^2\int_0^\infty j_l(kr)\,\Phi_l^l(r)\,V(r)\,r^2\,dr + 2\alpha\beta\int_0^\infty j_l(kr)\,\Phi_l^{l+1}(r)\,V(r)\,r^2dr + \beta^2\int_0^\infty j_{l+1}(kr)\,\Phi_{l+1}^{l+1}(r)\,V(r)\,r^2dr\right\},$$

$$\tan \delta_l^{(2)} = -\left(\frac{kK}{c\hbar}\right)\left\{\alpha \int_0^\infty j_l^2(kr) V(r) r^2 dr + \beta \int_0^\infty j_{l-1}^2(kr) V(r) r^2 dr\right\}$$
$$-\left(\frac{kK}{c\hbar}\right)^2 \left\{\alpha^2 \int_0^\infty j_l(kr)\, \Phi_l^l(r) V(r) r^2 dr + 2\alpha\beta \int_0^\infty j_l(kr)\, \dot{\Phi}_l^{l-1}(r) V(r) r^2 dr + \beta^2 \int_0^\infty j_{l-1}(r)\, \dot{\Phi}_{l-1}^{l-1}(r) V(r) r^2 dr\right\}. \quad (23)$$

From (23) we can obtain previous results as special cases. For example, neglecting the terms quadratic in $V(r)$, we get the results found from the damping theory for the scattering of Dirac particles, Eq. (19). In the case of small values of the scattering phase shifts $(\tan \delta_l \approx \delta_l)$ we find the results of the first Born approximation (cf. reference 3)

$$\delta_l^{(1)} = -\left(\frac{kK}{c\hbar}\right)\left\{\alpha \int_0^\infty j_l^2(kr) V(r) r^2 dr + \beta \int_0^\infty j_{l+1}^2(kr) V(r) r^2 dr\right\},$$
$$\delta_l^{(2)} = -\left(\frac{kK}{c\hbar}\right)\left\{\alpha \int_0^\infty j_l^2(kr) V(r) r^2 dr + \beta \int_0^\infty j_{l-1}^2(kr) V(r) r^2 dr\right\}.$$

The formulas in (23) can also be used to study the scattering by a center of Coulomb forces $(V(r) = -Ze^2/r)$. In this case it must be noted that the integrated values of the phase shifts diverge. Nevertheless, we get correct results if in the formulas (2) we first carry out the summation over l, which gives the following values for the scattering amplitudes in second approximation:

$$f(\theta) = \left(\frac{Ze^2}{c\hbar}\right)\frac{K}{8k^2}\left(\frac{2\alpha}{\sin^2(\theta/2)} + \frac{2\beta\cos\theta}{\sin^2(\theta/2)}\right) + \left(\frac{Ze^2}{c\hbar}\right)^2 \frac{\pi K^2}{4k^3}\frac{\alpha\beta}{\sin(\theta/2)}\left(1 - \sin\frac{\theta}{2}\right),$$
$$g(\theta) = \left(\frac{Ze^2}{c\hbar}\right)\frac{K}{8k^2}\frac{4\beta\cos(\theta/2)}{\sin(\theta/2)} + \left(\frac{Ze^2}{c\hbar}\right)^2 \frac{\pi K^2}{4k^3}\frac{\alpha\beta}{\cos(\theta/2)}\left(1 - \sin\frac{\theta}{2}\right).$$

From this we get for the differential cross section the well known formula which takes into account not only relativistic and spin effects but also terms of the second order in $V(r)$, which characterize the asymmetry of the scattering of electrons and positrons[4]

$$\frac{d\sigma}{d\Omega} = \left(\frac{Ze^2}{2mc^2}\right)^2 \frac{1 - v^2/c^2}{v^4/c^4}\sec^4\frac{\theta}{2}\left[1 - \frac{v^2}{c^2}\sin^2\frac{\theta}{2} + Z\pi\frac{v}{c}\left(\frac{e^2}{c\hbar}\right)\sin\frac{\theta}{2}\left(1 - \sin\frac{\theta}{2}\right)\right].$$

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