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Elastic scattering of neutrons by deuterons

By Gita Purkayastha and N. C. Sil

Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta-32

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The elastic scattering of neutron by deuteron has been investigated considering the exchange collision possibility. We have used a modification of the Born approximation due to Dirac which takes account of the non-orthogonality of the initial and final wave functions. The resulting integral equations have been solved by the Fredholm method. The calculations have been done for energies 60 Mev, 95 Mev. and 146 Mev of the incident neutrons. The results of our numerical calculation at 95 Mev are in good agreement with the experimental findings as well as the theoretical results of Wu & Ashkin. The non-orthogonality corrections are quite perceptible at lower energies but small at high energy.

Introduction

A number of theoretical calculations have been made by several authors (Massey & Buckingham 1941, Wu & Ashkin 1948, Chew 1948, Gammel & Christian 1953, Aron *et al* 1964, 1965) on the elastic scattering of neutrons and protons by deuterons. The Born approximation calculation which can be used for high energy of the incident particles deserves special consideration in view of its simplicity. However the exchange collision process brings in additional complications and the conventional Born-Oppenheimer approximation needs modification to take account of the lack of orthogonality of the initial and final states. Dirac (1955) has suggested a modification of Born-Oppenheimer approximation which is applicable in such cases. According to Dirac, in the transition problems for which the initial and final states belong to two different sets of orthogonal states, one has to deal with a mixture of wave functions belonging to two different orthogonal sets. It then becomes necessary to to take into account the lack of orthogonality of these wave functions. In this paper we have studied the elastic scattering, including exchange, of high energy neutrons by target deuteron in ground states by taking proper account of the non-orthogonality of the wave functions as suggested by Dirac, as in this case initial and final states are non-orthogonal. In view of the fact that there is no excited bound state of deuteron, we have considered only the following two possibilites, (1) that the incident neutron is scattered leaving the target in the ground state, (2) that the neutron bound originally in the deuteron comes out and the incident neutron is captured by the proton left to form a deuteron, in the ground state. The dissociation reaction in which the deuteron breaks up into a neutron and a proton has been neglected. By taking properly weighted symmetric and anti-symmetric combinations of the direct and exchange scattering amplitudes in the differential crosssection we make allowance for the indistinguishability of the incident neutron and the neutron in the target deuteron.

Formulations

Let 1 denote the incoming neutron, 3 and 2 are respectively the proton and the neutron originally forming the deuteron. Let us introduce the relative co-ordinate

$$\mathbf{r} = \mathbf{r}_1 - \frac{1}{2}\left(\mathbf{r}_2 + \mathbf{r}_3\right)$$

$$\mathbf{r}' = \mathbf{r}_2 - \frac{1}{2}\left(\mathbf{r}_1 + \mathbf{r}_3\right)$$

$$\rho = \mathbf{r}_3 - \mathbf{r}_2$$

$$\rho' = \mathbf{r}_3 - \mathbf{r}_1$$

We have assumed the centre of mass at rest i. e.

$$\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3 = 0.$$

We have considered only the following two probable reactions, (1) the incident neutron is scattered leaving the deuteron in its ground state (2) the exchange collision reaction i.e. the incident neutron is captured by the target to form a deuteron and the neutron which was originally in the target comes out. In the exchange collision process, the initial and the final wave functions are non-orthogonal as they are wave functions of two different Hamiltonians. The initial Hamiltonian is

$$H = H\,(D_{2,3}) + H\,(n_1) + V_1$$

The final Hamiltonian is

$$\bar{H} = H\,(D_{1,3}) + H\,(n_2) + V_2$$

where H $(D_{2,3})$ and H $(D_{1,3})$ are the energies of the deuteron formed of particles (2,3) and (1,3) respectively H (n_1) and H (n_2) are energies of the neutron 1 and the neutron 2. V_1 is the interaction energy between $(D_{2,3})$ and n_1 and V_2 is is the interaction energy between $(D_{1,3})$ and n_2.

The scattering and exchange collision reaction amplitudes, denoted respectively by $a(\mathbf{k})$ and $b(\mathbf{k})$ are given by Dirac as

$$a(\mathbf{k}) = -\int \psi_k{}^* \mid V_{12} + V_{13} \mid \psi_{k0}\, dq - \int w(\mathbf{k},\mathbf{k}')\, b(\mathbf{k}')\, d_k{}'$$

$$b(\mathbf{k}) = -\int \psi_k{}'^* \mid V_{21} + V_{23} \mid \psi_{k\,0}\, dq - \int w(\mathbf{k},\mathbf{k}')\, a(\mathbf{k})\, d_k$$

where $w(\boldsymbol{k},\boldsymbol{k}') = \int \psi_k^* \, \psi_k' \, dq$

$w(\boldsymbol{k}',\boldsymbol{k}) = \int \psi_k'^* \, \psi_k \, dq = w(\boldsymbol{k},\boldsymbol{k}')$

$dq = r^2 \sin\theta \, d\theta \, d\phi \, dr \, \rho^2 \sin\theta' \, d\theta' \, d\phi' \, d\rho$

and V_{12}, V_{13}, V_{21} and V_{23} are two body interaction potentials between particles (1,2), (1,3), (2,1) and (2,3) respectively. ψ_{k_0}, ψ_k and ψ_k' are the wave functions of the system at the beginning, after elastic scattering and after exchange collision process respectively. They are the products of deuteron bound state wave function and neutron wave function in relative co-ordinate multiplied by proper normalizing constant. The calculations have been carried out omitting tensor forces. The spin-orbit effect is also neglected. We have taken the radial part of the interaction potential as well as the state functions as of Gaussian nature. This particular form of potentials and state functions are simple in nature and enables us to do the calculation analytically. Thus we have

$$V_{ij} = V_0 \exp(-\alpha^2 r_{ij}^2) \qquad \ldots(a)$$

$$\left.\begin{aligned} \psi_k &= A \exp(i\,\boldsymbol{k}\,\boldsymbol{r} - \lambda^2\rho^2) \\ \psi_{k_0} &= A \exp(i\,\boldsymbol{k}_0 . \boldsymbol{r} - \lambda^2\rho^2) \\ \psi_k' &= A \exp(i\,\boldsymbol{k}' . \boldsymbol{r}' - \lambda^2\rho'^2) \end{aligned}\right\} \qquad \ldots(b)$$

were V_0, α^2, A and λ^2 are constant. Putting these values of V_{ij}'s and ψ's in in (1) and (2) and integrating, we get finally

$$a(\boldsymbol{k}) = -f(\boldsymbol{k}) - \int w(\boldsymbol{k},\boldsymbol{k}')\, b(\boldsymbol{k}')\, d^3\boldsymbol{k}' \qquad \ldots(3)$$

$$b(\boldsymbol{k}) = -g(\boldsymbol{k}) - \int w(\boldsymbol{k},\boldsymbol{k}')\, a_k' \, d^3\boldsymbol{k}' \qquad \ldots(4)$$

where

$$f(\boldsymbol{k}) = c \exp(-\alpha_1)(\boldsymbol{k}_0 - \boldsymbol{k})^2$$

$$g(\boldsymbol{k}) = d_1 \exp[-\{\beta(\boldsymbol{k}_0 - \boldsymbol{k})^2 + \gamma(\boldsymbol{k}_0 + \boldsymbol{k})^2\}]$$

$$+ d_2 \exp[-\{\delta\left(\boldsymbol{k} + \frac{\boldsymbol{k}_0}{2}\right)^2 + \mu(2\boldsymbol{k}_0 + \boldsymbol{k})^2\}]$$

with

$$c = \frac{A^2 V_0}{2^{7/2}\alpha^3\lambda^3}, \quad \alpha_1 = \frac{8\lambda^2 + \alpha^2}{32\lambda^2\alpha^2}$$

$$d_1 = \frac{A^2 V_0}{8\pi^3(\lambda^2 + 2\alpha^2)^{3/2}}, \quad d_2 = \frac{A^2 V_0}{8\pi^3(\lambda^2 + \alpha^2)^{3/2}}$$

$$\beta = \frac{1}{32\lambda^2}, \quad \gamma = \frac{9}{16(2\lambda^2 + 4\alpha^2)}, \quad \delta = \frac{1}{4\lambda^2}$$

$$\mu = 1/16(\lambda^2 + \alpha^2)$$

$$w(\boldsymbol{k},\boldsymbol{k}') = \frac{A^2}{8\lambda^6} \exp\left[-\frac{1}{4\lambda^2}\left\{\left(\boldsymbol{k} + \frac{\boldsymbol{k}'}{2}\right)^2 + \left(\frac{\boldsymbol{k}}{2} + \boldsymbol{k}'\right)^2\right\}\right]$$

Using equation (4) for the value of $b\boldsymbol{k}$ in equation (3) we get

$$a(\boldsymbol{k}) = F_k + P \int W(\boldsymbol{k},\boldsymbol{k}'')\, a(\boldsymbol{k}'')\, d^3\boldsymbol{k}'' \qquad \ldots(5)$$

Similarly equation for $b(\boldsymbol{k})$ takes the form

$$b(\boldsymbol{k}) = G(\boldsymbol{k}) + P \int W(\boldsymbol{k},\boldsymbol{k}'')\, b(\boldsymbol{k}'')\, d^3\boldsymbol{k}'' \qquad \ldots(6)$$

where

$$F(\boldsymbol{k}) = -f(\boldsymbol{k}) + \int W(\boldsymbol{k},\boldsymbol{k}')\, g(\boldsymbol{k}')\, d^3\boldsymbol{k}'$$

$$G(\boldsymbol{k}) = -g(\boldsymbol{k}) + \int W(\boldsymbol{k},\boldsymbol{k}')\, f(\boldsymbol{k}')\, d^3\boldsymbol{k}'$$

$$P\, W(\boldsymbol{k},\boldsymbol{k}'') = \int W(\boldsymbol{k},\boldsymbol{k}')\, w(\boldsymbol{k}',\boldsymbol{k}'')\, d^3\boldsymbol{k}'.$$

More explicitly $P = \dfrac{A^4}{\lambda^9}\left(\pi/10\right)^{3/2}$.

$$W(\boldsymbol{k},\boldsymbol{k}'') = e - \left\{\frac{45}{272}\frac{k^2}{\lambda_2} + \frac{17}{125\lambda^2}\left(\frac{5}{4}k - \frac{10}{17}k\right)^2\right\}$$

$$\int w(\boldsymbol{k},\boldsymbol{k}')\, g(\boldsymbol{k}')\, d^3\boldsymbol{k}' = N e^{-9/80(k/\lambda)^2} \qquad \ldots(7)$$

where
$$N = \frac{8d_1A^2}{\lambda^3}\left(\frac{\pi}{5+16\lambda^2(\beta+\gamma)}\right)^{3/2}$$

$$\times \exp\left[-\left\{\frac{\beta\gamma}{\beta+\gamma}\, 4\boldsymbol{k}_o^2 + \frac{5(\beta+\gamma)}{5+16\lambda^2(\beta+\gamma)}\left(\frac{\boldsymbol{k}_o(\beta-\gamma)}{\beta+\gamma} + \frac{4}{5}\boldsymbol{k}\right)^2\right\}\right]$$

$$+ 8\,\frac{d_2A^2}{\lambda^3}\left(\frac{\pi}{5+16\lambda^2(\delta+\mu)}\right)^{3/2}$$

$$\times \exp\left[-\left\{\frac{\delta\mu}{\delta+\mu}\,\frac{9}{4}\,\boldsymbol{k}_o^2 + \frac{5(\delta+\mu)}{5+16\lambda^2(\delta+\mu)}\left(\frac{\boldsymbol{k}_o(\delta+4\mu)}{2\delta+2\mu} - \frac{4}{5}\boldsymbol{k}\right)^2\right\}\right]$$

and
$$\int w(\boldsymbol{k},\boldsymbol{k}')\, f(\boldsymbol{k}')\, d^3\boldsymbol{k}' = M \exp\left[-\frac{9}{80}\left(\frac{\boldsymbol{k}}{\lambda}\right)^2\right] \qquad \ldots(8)$$

where
$$M = \frac{C\,A^2}{8\,\lambda^6}\left(\frac{\pi 16\lambda^2}{5+16\,\lambda^2\,\alpha_1}\right)^{3/2} \times \exp\left[-\frac{5\alpha_1}{5+16\alpha_1\lambda^2}\left(\frac{4}{5}\boldsymbol{k} + \boldsymbol{k}_o\right)^2\right]$$

The integral equations (5) and (6) cannot be solved by successive approximation method as the resulting series are not convergent. We have solved them by Fredholm method. We attempted to solve (5) and (6) by means of a power series in P

$$a(\boldsymbol{k}) = \sum_{n=0}^{\infty} P^n\, a_n(\boldsymbol{k})\ ; \ldots (9) \qquad b(\boldsymbol{k}) = \sum_{n=0}^{\infty} P^n\, b_n(\boldsymbol{k}) \qquad (10)$$

Substituting (9) and (10) in (5) and (6)

$$a(\boldsymbol{k}) = \sum_{n=0}^{\infty} P^n\, a_n(\boldsymbol{k}) = F(\boldsymbol{k}) + P\int w(\boldsymbol{k},\boldsymbol{k}') \sum_{n=0}^{\infty} P^n\, a_n(\boldsymbol{k}')\, d^3\boldsymbol{k}' \qquad \ldots(11a)$$

$$b(\boldsymbol{k}) = \sum_{n=0}^{\infty} P^n \, b_n(\boldsymbol{k})$$

$$= G(\boldsymbol{k}) + P \int w(\boldsymbol{k},\boldsymbol{k}'') \sum_{n=0}^{\infty} P^n \, b_n(\boldsymbol{k}'') \, d^3\boldsymbol{k}''. \qquad \text{...(11b)}$$

Equating coefficients of equal power of P we obtain

$$a_0(\boldsymbol{k}) = F(\boldsymbol{k})$$

$$a_1(\boldsymbol{k}) = \int W(\boldsymbol{k},\boldsymbol{k}'') \, a_0(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

$$a_2(\boldsymbol{k}) = \int W(\boldsymbol{k},\boldsymbol{k}'') \, a_1(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

$$a_n(\boldsymbol{k}) = \int W(\boldsymbol{k},\boldsymbol{k}'') \, a_{n-1}(\boldsymbol{k}'') \, d^3\boldsymbol{k}''. \qquad \text{...(12)}$$

Similarly for $b(\boldsymbol{k})$'s we get

$$b_0(\boldsymbol{k}) = G(\boldsymbol{k})$$

$$b_1(\boldsymbol{k}) = \int W(\boldsymbol{k},\boldsymbol{k}'') \, b_0(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

$$b_n(\boldsymbol{k}) = \int W(\boldsymbol{k},\boldsymbol{k}'') \, b_{n-1}(\boldsymbol{k}'') \, d^3\boldsymbol{k}''. \qquad \text{...(13)}$$

In order to obtain the solution in more convenient form, we define the iterated kernels

$$W_1(\boldsymbol{k},\boldsymbol{k}'') = W(\boldsymbol{k},\boldsymbol{k}'')$$

$$W_2(\boldsymbol{k},\boldsymbol{k}'') = \int W(\boldsymbol{k},\boldsymbol{k}') \, w(\boldsymbol{k}',\boldsymbol{k}'') \, d^3\boldsymbol{k}'$$

$$W_n(\boldsymbol{k},\boldsymbol{k}'') = \int W_{n-1}(\boldsymbol{k},\boldsymbol{k}') \, w(\boldsymbol{k}',\boldsymbol{k}'') \, d^3\boldsymbol{k}' \qquad \text{...(14)}$$

$$a_0(\boldsymbol{k}) = F(\boldsymbol{k})$$

$$a_1(\boldsymbol{k}) = \int W_1(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

$$a_2(\boldsymbol{k}) = \int W_2(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

$$a_n(\boldsymbol{k}) = \int W_n(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}''.$$

Also the equations for the $b(\boldsymbol{k})$'s can be obtained by writing $G(\boldsymbol{k})$ instead of $F(\boldsymbol{k})$

$$a(\boldsymbol{k}) = F(\boldsymbol{k}) + P \int W_1(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}'$$

$$+ P^2 \int W_2(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}'' + P^3 \int W_3(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}'' + \ldots$$

$$= F(\boldsymbol{k}) + P \int \Sigma P^n \, W_{n+1}(\boldsymbol{k},\boldsymbol{k}'') \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

$$= F(\boldsymbol{k}) + P \int W(\boldsymbol{k},\boldsymbol{k}'' ; P) \, F(\boldsymbol{k}'') \, d^3\boldsymbol{k}''$$

where $W(\boldsymbol{k},\boldsymbol{k}'' ; P) = \sum_{n=0}^{\infty} P^n W_{n+1}(\boldsymbol{k},\boldsymbol{k}'')$.

Similarly

$$b(\boldsymbol{k}) = G(\boldsymbol{k}) + P \int W(\boldsymbol{k},\boldsymbol{k}'' ; P) \, G(\boldsymbol{k}'') \, d^3\boldsymbol{k}''.$$

In Fredholm method of solution the resolvent is the ratio of two infinite series in P.

$$W(\boldsymbol{k},\boldsymbol{k}'';P) = \frac{D(\boldsymbol{k},\boldsymbol{k}'';P)}{D(P)}$$

where

$$D(\boldsymbol{k},\boldsymbol{k}'';P) = W(\boldsymbol{k},\boldsymbol{k}'') + \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} D_n(\boldsymbol{k},\boldsymbol{k}'') P^n$$

$$D(P) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} D_n P^n.$$

The coefficients D_n and the functions $D_n(\boldsymbol{k},\boldsymbol{k}'')$ may be found from the following recurrence relations

$$D_m(\boldsymbol{k},\boldsymbol{k}'') = W(\boldsymbol{k},\boldsymbol{k}'') D_m - m\int W(\boldsymbol{k},\boldsymbol{k}') D_{m-1}(\boldsymbol{k}',\boldsymbol{k}'')\, d\boldsymbol{k}'$$

where

$$D_m = \int D_{m-1}(\boldsymbol{k},\boldsymbol{k})\, d\boldsymbol{k} \quad \text{and} \quad W(\boldsymbol{k},\boldsymbol{k}'') = D_0(\boldsymbol{k},\boldsymbol{k}''),$$

Using the above recurrence relation we get

$$a(\boldsymbol{k}) = -\frac{F(\boldsymbol{k}) + P\displaystyle\int\left[W(\boldsymbol{k},\boldsymbol{k}'') + \sum_{n=1}^{\infty}\frac{(-1)^n}{n!}P^n\left\{W(\boldsymbol{k},\boldsymbol{k}'')D_n - n\int W(\boldsymbol{k},\boldsymbol{k}') D_{n-1}(\boldsymbol{k}',\boldsymbol{k}'')d^3\boldsymbol{k}'\right\}\right]F(\boldsymbol{k}'')\,d^3\boldsymbol{k}''}{\displaystyle\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}D_n P^n}.$$

and a similar equation for $b(\boldsymbol{k})$'s.

We have taken upto seven order for the expansion of $a(\boldsymbol{k})$ and $b(\boldsymbol{k})$ as the seventh term is found to be sufficiently small. Making allowance for the indistinguishability we may have the differential cross-section as

$$d\sigma(\theta) = \frac{14\pi^2\mu^2}{\hbar^4}\left[\left\{\frac{1}{4}\left|a_k(\theta) + b_k(\theta)\right|^2 + \frac{3}{4}\left|a_k(\theta) - b_k(\theta)\right|^2\right\}\right]$$

where $a_k(\theta) = a(\boldsymbol{k})$ at θ ; $b_k(\theta) = b(\boldsymbol{k})$ at θ,

Numerical calculations have been done using I.B.M. 1620 computer.

Results and Disscussions

We have calculated the disfferential cross section for elastic scattering at different energies of the incident neutron. The radial part of the two body interaction potentials and wave function of bound state of deuteron are taken to be of Gaussian type (cf. equations (a) and (b)). The values of the parameters used are (Wu & Ashkin 1948)

$$V_0 = 45 \text{ Mev} \qquad \kappa^2 = \cdot 266 \times 10^{26}\text{cm}^{-2}$$

$$A = 0.312 \times 10^{19}\text{cm} \qquad \lambda^2 = \cdot 0716 \times 10^{26}\text{cm}^{-2}.$$

The curves are drawn showing differential cross sections against scattering angles in centre of mass system at 60 Mev, 95 Mev and 146 Mev (figures 1—3). The results at 95 Mev and 146 Mev are compared with the experimental findings of Chamberlain & Stern (1954), Cassels *et al* (1951) and with the results of theoretical calculations of Wu & Ashkin (1948). We have further added a table which gives the direct elastic and exchange collision amplitudes in Born approximation and also their modification due to the lack of orthogonality effect at those energies.

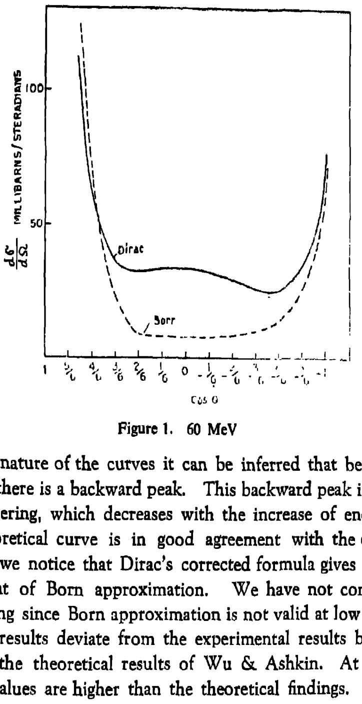

Figure 1. 60 MeV

From the nature of the curves it can be inferred that besides a sharp forward peak there is a backward peak. This backward peak is due to the exchange scattering, which decreases with the increase of energy. At 95 Mev our theoretical curve is in good agreement with the experimental curves. Here we notice that Dirac's corrected formula gives better agreement than that of Born approximation. We have not considered low energy scattering since Born approximation is not valid at low energy. At 146 Mev our results deviate from the experimental results but agree reasonably with the theoretical results of Wu & Ashkin. At this energy, experimental values are higher than the theoretical findings. However, it should be mentioned that in such range of energy the deuteron disintegration probability is quite appreciable which has not been taken into account in our formulation. It is also neglected in the formulation of Wu & Ashkin. Further in both the theoretical formulations the spin orbit forces have been neglected which may have appreciable contribution at such energies. From the curves as well as from the table it is clear that the non-

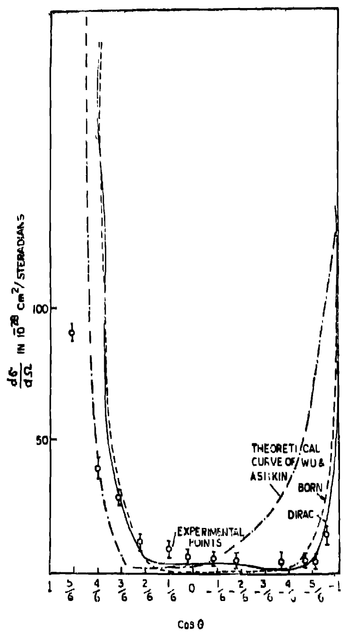

Figure 2. 95 MeV

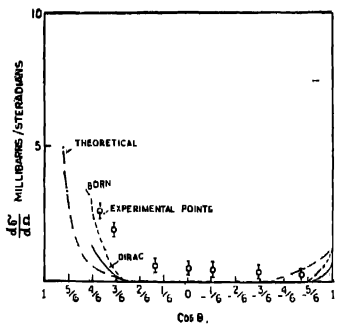

Figure 3. 146 MeV

TABLE 1

	Energy/Cosθ	−1	−2/3	−1/3	0	1/3	2/3	1
$a_k(\theta)$ in 10^{-15} cm	Born 60 Mev	.02037	.066	.2139	693	2.2456	7.276	23.5765
	Dirac's correction	−.0677	−.12	−.2513	−.3738	−.353	−.4325	−.8822
$b_k(\theta)$ in 10^{-15} cm	Born	7.012	2.9789	2.639	2.482	2.436	2.2094	1.8061
	Dirac's correction	−.0587	1.0854	1.687	2.3102	2.7114	3.0113	3.8143
$a_k(\theta)$ in 10^{-15} cm	Born 95 Mev	.00033	.00214	.0137	.08856	.5697	3.665	23.5765
	Dirac's correction	−.00994	−.0136	−.0275	−.0348	−.0289	−.042	−.1688
$b_k(\theta)$ in 10^{-15} cm	Born	2.983	.4198	.265	.243	.237	.2276	.2186
	Dirac's correction	−.9008	−.087	.1997	.2467	.3266	.374	.4168
$a_k(\theta)$ in 10^{-15} cm	Born 146Mev	$.8\times10^{-6}$	$.1455\times10^{-4}$	.00026	.0044	.0775	1.3512	23.5765
	Dirac's correction	−.00065	−.000734	−.001	−.00129	−.0009	−.00218	−.0209
$b_k(\theta)$ in 10^{-15} cm	Born	.8925	−.049	.0365	.0342	.0322	.0303	.0285
	Dirac's correction	−.1959	−.029	.00102	.00669	.0085	.01006	.0125

$a_k(\theta)$=direct elastic scattering amplitude at θ

$b_k(\theta)$=exchange elastic scattering amplitude at θ

orthogonality effect decreases the increase of energy. At 60 Mev and 90 Mev this effect is quite significant whereas at 146 Mev this effect is much less.

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