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The Dependenceon Energy of Scattering Cross-Section By Spherical Square Well Potential Using Born's Approximation

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Abstract

Using Born's approximation techniques, to investigate the dependence on energy of scattering cross-section by spherical square well potential, an analytical expression for the differential scattering cross section has been calculated and energy limits were obtained.The dependence on energy of scattering cross-section in the low and high energy limits were examined by computing numerical values of the scattering function. Graphical plots were also obtained to check the pictorial representation of scattering cross-section.The study has shown that Born's approximation is only applicable in the high energy limit where the potential is weak. It indicates that the potential is strong enough to bind a particle, thus Born approximation cannot be applied in the low energy limit and in the scattering at low energies.

1.0 Introduction

Whenever a beam of particles of any kind is directed at matter, the particles will be deflected out of their original paths as a result of collision with the particles of matter which they encounter, and the process is known as scattering [1]. The problem of studying scattering process is important for two reasons; firstly, a great many interesting effects such as the stopping electrons in gaseous discharges, the collision determined, at least in part, by the probability of scattering; secondly, the fact that from the detailed study of the results of scattering, much can be learnt about the nature of particles that are being scattered, and as well as those that are doing the scattering. [2].
Scattering theory has found vast number of applications, such as echolocation, geophysical survey, non destructive testing, medical imaging, cross-section calculations and quantum field theory [3]. Born approximation is used to show the dependence on energy of scattering cross section by spherical square well potential, which shows the difference in the low and high energy limits.One can also showwhere Born'sapproximation can be applied and where it cannot be applied if the potential is too weak or too strong.Scattering cross section is of paramount importance in nuclear physics. The study of the dependence of scattering cross-section by spherical square well potential using Born's approximation goes a long way in understanding nuclear cross section and cross section calculations.
This study will therefore help in understanding the concepts of scattering by spherical square well potential, cross-sections or nuclear cross-sections and Born's approximation. Also the comparison between theory and numerical analysis will be appreciated.

2.0 Theory

Scattering by a square well potential

The zero energy scattering can be characterized by just one parameter, the scattering length. As the energy is increased, more and more of the partial waves would begin to get scattered and in turn making scattering dependent both on energy and the scattering angle. If the energy is only slightly higher than the zero energy, the energy dependence makes its appearance. This energy can be described in terms of a parameter called effective range. It can be illustrated in the case of scattering by a short range attractive square well potential which is displayed in Fig.1and represented mathematically as

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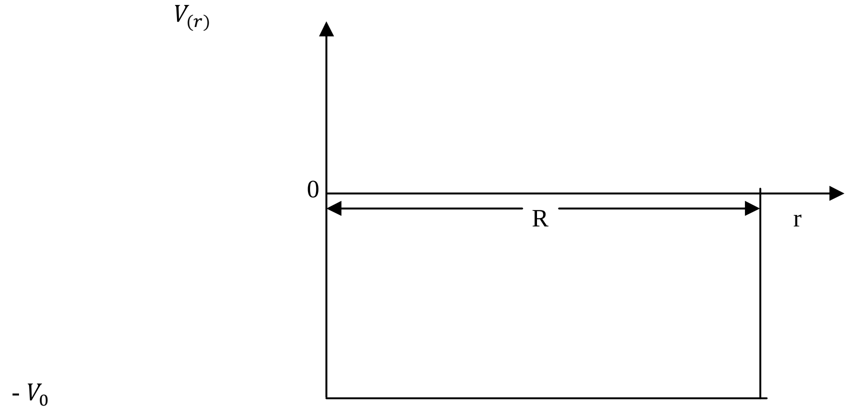

Fig. 1: Square well potential.

$$V(r) = \begin{cases} -V_0, & r < R \\ 0, & r > R \end{cases} \quad (1)$$

It is known that the radial part of Schrodinger equation in the presence of scattering potential V(r) for $l = 0$, is given by

$$\frac{1}{r^2}\frac{d}{dr}\left(\frac{r^2 d\Psi_o}{dr}\right) + [k^2 - U(r)]\Psi_o = 0 \quad (2a)$$

Where $k^2 = \frac{2\mu E}{\hbar^2}$, $U(r) = \frac{2\mu V(r)}{\hbar^2}$ (2b)

After substituting$\Psi_o(r) = \frac{F(r)}{r}$, the above equation takes the form

$$\frac{d^2F(r)}{dr^2} + k^2 F(r) = 0\,, \quad r < R \quad (3a)$$

with $k^2 = K^2 + K_0^2$, $K_0^2 = \frac{2\mu V_0}{\hbar^2}$ (3b)

Similarly putting $U(r) = 0$ in equation (2) and further substituting,

$\Psi_o^o(r) = \frac{F(r)}{r}$,where zero in the superscript of Ψ_o $r$represents radial solution, in the absence of V(r), we get

$$\frac{d^2f(r)}{dr^2} + k^2 f(r) = 0\,, \quad r>R \quad (4)$$

The Schrodinger's equation to be solved for the Born's approximation, for a spherically symmetric potential, can be cast in its differential form as

$$\nabla^2\varphi(r) + \frac{2\mu}{\hbar^2}[E - V(r)]\varphi(r) = 0 \quad (5)$$

Or, $(-\nabla^2 - k^2)\varphi(r) = U(r)\varphi(r)= F(r)$

On application of Green's functions, the differential equation (5) becomes

$$\varphi(r)\overrightarrow{r \to \infty} e^{ikz} - \frac{1}{4\pi}\frac{e^{ikr}}{r}\int e^{-ikn.r}\,\varphi(r)U(r)dr \quad (6)$$

Equation (6) implies that the second term is the product of an outgoing spherical wave $\frac{e^{ikr}}{r}$ and some angular amplitude independent of r. Thus the scattered amplitude in the Born approximation will be given by

$$f(\theta,\emptyset) = -\frac{1}{4\pi}\int e^{-ikn.r}\varphi(r)U(r)dr \quad (7)$$

We now use the Born approximation method to solve equation (7).

In the zeroth approximation, we neglect the integral term in equation (7) and set $\varphi(r) = \varphi^0(r) = e^{ikz}$, then we use the zeroth approximation on the right hand side of equation 6 to compute the first Born approximation, $\varphi^1(r)$. Thus we have

$$\varphi(r) = \varphi^1(r) = e^{ikz} - \frac{1}{4\pi}\frac{e^{ikr}}{r}\int e^{-ikn.r}e^{ikz}U(r)dr \quad (8)$$

Insert $\varphi^1(r)$ on the right hand side of (8) to compute the second approximation $\varphi^2(r)$ and so on. The n^{th} approximation is

$$\varphi^n(r) = e^{ikz} - \frac{1}{4\pi}\frac{e^{ikz}}{r}\int e^{-ikn.r}\varphi^{(n-1)}(r)U(r)dr \quad (9)$$

Thus in the general case where V(**r**) ≠ V(r), the scattered amplitude in the first Born approximation would be given by

$$f(\theta,\emptyset) = -\frac{1}{4\pi}\int e^{-ikn.r}e^{ikz}U(r)dr \quad (10)$$

Let $\mathbf{k_0}$ be a vector of magnitude k that has direction of the incident beam (polar axis), **k** is the vector of magnitude k for the scattered particle and θ is the angle of scattering. Note that the magnitudes k_0 and k are the same since the scattering is elastic. Thus $e^{ikz}= e^{-ik_0.r}$. Substitute this in the above equation to obtain

$$f(\theta,\emptyset) = -\frac{1}{4\pi}\int e^{i(k_0-k).r}U(r)dr = -\frac{1}{4\pi}\int e^{iK.r}U(r)dr \quad (11)$$

where**K** = $\mathbf{k}_0$–**k**as shown in Fig.1**.**This is Fourier transform of the scattering potential.

The magnitude of **K**is $[(\mathbf{k}_o-\mathbf{k}).(\mathbf{k}_o-\mathbf{k}) = \{2k^2(1-\cos\theta)\}^{\frac{1}{2}} = 2k\sin(\theta/2)]$. Its physical significance is that ħK is the momentum transferred to the particle in its encounter with the potential. **K** is the momentum transfer vector.

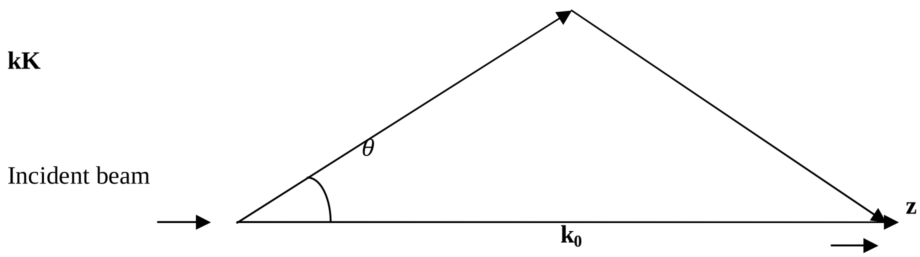

Fig. 2: The incident wave vector $\mathbf{k}_0$, the scattered wave vector **k,** and the transferred wave vector **K**

The differential scattering cross section in the Born approximation is

$$\sigma(\theta,\emptyset) = |f(\theta,\emptyset)|^2 = \left(\frac{1}{4\pi}\right)^2 \left|\int e^{iK.r}U(r)dr\right|^2 \qquad (12)$$

For a central force, V(**r**) = V(r). In the majority of practical situations, we deal with central forces. Thus the scattering amplitude, equation (11), in this case would be

$$f(\theta) = \ -\frac{1}{4\pi}\int e^{iK.r}U(r)dr, \qquad (13)$$

where**K** depends on θ. The integrand being scalar, the integral will be independent of the coordinate system in which it is evaluated. Integrating in polar spherical coordinate system, we get

$$f(\theta) = -\frac{1}{4\pi}\int_0^\infty \int_0^\pi \int_0^{2\pi} e^{iKr\cos\alpha}U(r)\, r^2 \sin\alpha\, dr\, d\alpha\, d\beta \qquad (14a)$$

Where (r,α,β) define the position of particle with respect to the K – axis as the polar axis. This results to

$$f(\theta) = -\frac{1}{K}\int_0^\infty r\sin Kr\, U(r)dr \qquad (14b)$$

Hence the differential scattering cross section will be given by

$$\sigma(\theta) = |f(\theta)|^2 = \frac{1}{K^2}\left|\int_0^\infty r\sin Kr\, U(r)dr\right|^2 \qquad (15)$$

Equation (14)implies that $\sigma(\theta)$ is independent of $\emptyset$ (as expected) and depends on θ through K and not on the momentum of incident particle or on scattering angle individually.

2.0 Validity of born approximation- case of square well potential

In obtaining equation (8) we replaced $\varphi(r)$ in the integral term by e^{ikz}. This is possible if Born approximation is to be valid, that is if the second term can be neglected in comparison with the first term, that is

$$|\varphi(r)| \ll \left|e^{ikz}\right| = 1 \qquad (16)$$

Where $\varphi(r) = -\frac{1}{4\pi}\int \frac{e^{ik|r-\acute{r}|}}{|r-\acute{r}|} e^{ikz}U(r)dr$ (17)

which depends on U(r) or effectively on V(r) which is appreciable near the origin for a short range potential. That is the value of $\varphi(r)$ would be largest near the origin (the centre of scattering potential at r = 0). Thus the validity condition becomes

$$|\varphi(0)| \ll 1 \qquad (18)$$

From equation 16 in the case of spherically symmetric potential, that is U(**r**) = U(r), we get

$$\varphi(0) = -\frac{1}{4\pi}\int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{e^{ikr}}{r} e^{ikz}U(r)r^2 \sin\theta\, dr\, d\theta\, d\emptyset \qquad (19)$$

Putting z = r$\cos\theta$ and integrating over the polar angles $(\theta,\emptyset)$ of r, we get

$$\varphi(0) = \frac{-1}{2ik}\int_0^\infty U(r)\left(e^{2ikr}-1\right)dr, \qquad (20)$$

$U(r) = \frac{2\mu V(r)}{\hbar^2}$and $V(r) = V_0$.

The validity condition using equation (16) and (20), and the relation $U(r) = \frac{2\mu V(r)}{\hbar^2}$, becomes

$$\frac{\mu}{\hbar^2 k}\left|\int_0^R V(r)\left(e^{2ikr}-1\right)dr\right| \ll 1 \qquad (21)$$

We shall analytically determine the dependence of the cross section on the energy by examining the scattering amplitude of the attractive square well potential, V(r).

3.0 Methodology

The method that will be used for the dependence of energy of scattering cross-section by spherical square well potential is the Born approximationbysolving for the analytical resultwhich will be used to obtain the scattering cross- section (σ) that will enable one to obtain the energies in the lower and higher limits, whichin turn will show the dependence on energy of scattering cross-sections.

An attractive square well potential is represented by equation (1), where the scattering amplitude in this case is given by

$$f(\theta) = -\frac{1}{K}\int_0^{\infty} rU(r)\sin Kr dr \tag{22}$$

where K = 2ksin $\frac{\theta}{2}$.

Substituting the value of U(r) in equation (2b) into equation (22) gives

$$f(\theta) = \frac{-1}{K}\int_0^{\infty} r\frac{2\mu V(r)}{\hbar^2}\sin Kr dr \tag{23}$$

Using equation (1) into equation (23)

$$f(\theta) = \frac{2\mu V_0}{\hbar^2 K}\int_0^{R} r\sin Kr dr \tag{24}$$

Integrating equation (24) by partsgives

$$f(\theta)=\frac{2\mu V_o}{\hbar^2 K^3}(\sin KR - KR\cos KR) \tag{25}$$

The differential scattering cross-section is

$$\sigma(\theta)=|f(\theta)|^2 \tag{26}$$

Using (22) in (26),

$$\sigma(\theta)=[\frac{2\mu V_o}{\hbar^2 K^3}\ (\sin KR - KR\cos KR)]^2$$

Substitute x = KR =2kR$\sin\frac{\theta}{2}$, to obtain

$$\sigma(\theta) = (\frac{2\mu V_0 R^3}{\hbar^2})^2(\frac{\sin x - x\cos x}{x^3})^2 \tag{27}$$

Let $$(\frac{\sin x - x\cos x}{x^3})^2 = g(x) \tag{28}$$

$$\sigma(\theta)= (\frac{2\mu V_0 R^3}{\hbar^2})^2\ g(x) \tag{29}$$

Further, the total scattering cross-section would be given by

$$\sigma_t=(\frac{2\mu V_0 R^3}{\hbar^2})^2\int_0^{\pi}\int_0^{2\pi}(\frac{\sin x - x\cos x}{x^3})^2 \sin\theta d\theta\, d\phi \tag{30}$$

Since x = 2kR sin$\frac{\theta}{2}$, dx= 2kR$\frac{1}{2}\cos\frac{\theta}{2}d\theta$ and xdx= $(kR)^2\sin\theta d\theta$.

Or $\sin\theta d\theta = \frac{xdx}{(kR)^2}$

Thus, $\sigma_t=(\frac{2\mu V_0 R^3}{\hbar^2})^2\int_0^{\pi}(\frac{\sin x - x\cos x}{x^3})^2\sin\theta\, d\theta\int_0^{2\pi} d\phi$

$$\sigma_t=(\frac{2\mu V_0 R^3}{\hbar^2})^2 2\pi\int_0^{\pi}\frac{(\sin x - x\cos x)^2}{x^6}\frac{1}{(kR)^2}xdx$$

Substituting y = 2kR and changing π to y

$\sigma_t=\frac{32\pi\mu^2 V_0^2 R^6}{\hbar^4}\int_0^{y}\frac{(\sin x - x\cos x)^2}{x^5}\frac{1}{y^2}dx = \frac{32\pi\mu^2 V_0^2 R^6}{\hbar^4}\gamma(y)$ (31a)where$\gamma(y)=\frac{1}{y^2}\int_0^{y}\frac{(\sin x - x\cos x)^2}{x^5}dx = \frac{1}{4y^2}\left(1-\frac{1}{y^2}+\frac{\sin 2y}{y^3}-\frac{\sin^2 y}{y^4}\right)$ (31b)

Equation (30) is the analytically calculated total cross section as seen by the Born approximation for the spherical square well potential. This will be used to determine the dependence of cross section on lower and higher energy limits.

4.0 Discussion of Results

(i) Cross section dependance on the low energy limit (kR<<1), k small

To see the dependence of $\sigma(x)$in the low energy limit, apply trigonometric expansion (ө in radians) to equation (28) to obtain

$$g(x) = \left|\frac{\left\{\left(x-\frac{x^3}{3!}\right)-x\left(1-\frac{x^2}{2!}\right)\right\}}{x^3}\right|^2 = \left[\frac{\left(1-\frac{1}{6}\right)-1\left(1-\frac{1}{2}\right)}{1^3}\right]^2 = \frac{1}{9} \tag{32}$$

or$g(0) = \frac{1}{9}$. Fig.3 shows the plot of the function $\frac{g(x)}{g(0)}$versus x. As ө increases x increases, since K increases, and therefore $g(x)$ decreases. The variation of $\frac{g(x)}{g(0)} = 9g(x)$ with x shows that at x=0, $\frac{g(x)}{g(0)}$ is unity but falls off rapidly and at x ~ 4, it is zero. At x = $\frac{3\pi}{2}$, $\frac{g(x)}{g(0)}$ = 0. The computed values are shown in Table 1.

Table 1: Differential scattering cross-section as a function of scattering angle.

X(Radian)	g(x)	g(0)(radian)	g(x)g(0)
0	$\frac{1}{9}$	$\frac{1}{9}$	1
$\frac{\pi}{2}$	0	0.14	0
$\frac{3\pi}{2}$	0	0.33	0
$\frac{5\pi}{2}$	0	0.33	0

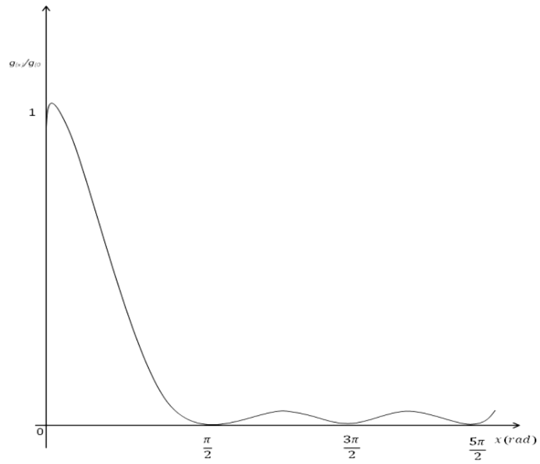

Fig. 3: The variation of $\frac{g(x)}{g(0)} = 9g(x)$ with x

The differential scattering cross section using equation (29) and (32) would be given by

$$\sigma(x) = \left(\frac{2\mu V_0 R^3}{\hbar^2}\right)^2 g(x) = \left(\frac{2\mu V_0 R^3}{\hbar^2}\right)^2 . \frac{1}{9}$$

$$\sigma_{diff} \xrightarrow[ksmall]{} \left(\frac{2\mu V_0 R^3}{3\hbar^2}\right)^2 \quad (33)$$

This infers that the scattering is isotropic (independent of scattering angle) at low energies

Now for $\gamma(y) = \gamma(0) = \frac{1}{18}$, the total cross-section at low energies from equation (31a) would be given by

$$\sigma_t = \frac{32\pi\mu^2 V_0^2 R^6}{\hbar^4} . \gamma(y) = \frac{32\pi\mu^2 V_0^2 R^6}{\hbar^4} . \frac{1}{18} = \frac{16\pi\mu^2 V_0^2 R^6}{9\hbar^4}, \text{ k R >> 1, k large} \quad (34)$$

(i) Dependance of cross section in the high energy limit

In the high energy limit (kR>> 1), x would increase much faster than $sinx$ as the maximum value of $sinx$ is 1. Thus equation (28) becomes

$$g(x) = \left(\frac{-\cos x}{x^2}\right)^2 \quad (35)$$

Using this in equation (22)

$$\sigma(\theta) = \left(\frac{2\mu V_0 R^3}{\hbar^2}\right)^2 \left(\frac{-\cos x}{x^2}\right)^2 \quad (36)$$

Recall $x = 2kR\sin\frac{\theta}{2}$

$$\sigma(\theta) \xrightarrow[klarge]{} \left(\frac{2\mu V_0 R^3}{\hbar^2}\right)^2 \left(\frac{-\cos\left(2kRsin\frac{\theta}{2}\right)}{\left(2kRsin\frac{\theta}{2}\right)^2}\right)^2$$

$$\sigma(\theta) \xrightarrow[klarge]{} \left(\frac{2\mu V_0 R^3}{\hbar^2}\right)^2 \frac{cos^2\left(2kRsin\frac{\theta}{2}\right)}{\left(2kRsin\frac{\theta}{2}\right)^4}$$

$$\sigma(\theta) \xrightarrow[klarge]{} \left(\frac{\mu V_0 R}{2\hbar^2 k^2}\right)^2 cos^2\left(2kRsin\frac{\theta}{2}\right) cosec^4\frac{\theta}{2} \quad (37)$$

which fluctuates with θ, to get rid of the term $cos^2\left(2kRsin\frac{\theta}{2}\right)$ let us take its average value $\frac{1}{2}$[4]. Thus

$$\sigma(\theta) = \left(\frac{\mu V_0 R}{2\hbar^2 k^2}\right)^2 . \frac{1}{2} cosec^4\frac{\theta}{2} \quad (38)$$

$E = \frac{\hbar^2 k^2}{2\mu}$ is the bombarding energy in the centre of mass system

$$\sigma_{(\theta)} = \frac{1}{2}\left(\frac{V_0 R}{4E}\right)^2 cosec^4\frac{\theta}{2} \quad (39)$$

This result indicates that the scattering shows a strong maximum in the forward direction (θ = 0) at high energies.Now for y large andfrom equation (31b)

$$\gamma(y) = \frac{1}{4y^2} = \frac{1}{16k^2R^2} \quad (40)$$

Using equation (37) and the first of equation (2b) in equation (31a), the total scattering cross-section at large energies would be given by

$$\sigma(t) = \frac{32\pi\mu^2 V_0^2 R^6}{\hbar^4}\gamma_{(y)} = \frac{\mu\pi V_0^2 R^4}{\hbar^2 E} \quad (41)$$

From equation (21), the validity of Born approximation becomes

$$\frac{\mu V_0}{\hbar^2 k}\left|\int_0^R (e^{2ikr}-1)dr\right| \ll 1$$

$$\frac{\mu V_0}{2\hbar^2 k}\left|\left[\frac{e^{2ikr}}{ik}-r\right]\right| \ll 1$$

butkR=y

$$\frac{\mu V_0}{2\hbar^2 k^2}\left|e^{iy}-1-iy\right| \ll 1$$

$$\frac{\mu v_0}{2\hbar^2 k^2}\left|(cosy-1)+\ i(siny-y)\right| \ll 1 \qquad (42)$$

Multiplying the above equation (42) by its conjugate and taking the square root, one gets;

$$\frac{\mu v_0}{2\hbar^2 k^2}\left[(cosy-1)^2+\ (siny-y)^2\right]^{\frac{1}{2}} \ll 1 \qquad (43)$$

The low energy limit, that is for y small

From equation (42), we have:

$$[(cosy-1)^2+(siny-y)^2]^{\frac{1}{2}} \sim \left[\left(1-\frac{y^2}{2!}-1\right)^2+\left(y-\frac{y^3}{3!}-y\right)^2\right]^{\frac{1}{2}} = \left[\frac{y^4}{4}+\frac{y^6}{36}\right]^{\frac{1}{2}}$$

Neglecting $\frac{y^6}{36}$ in comparison to $\frac{y^4}{4}$ one gets; $\left[\frac{y^4}{4}\right]^{\frac{1}{2}} = \frac{y^2}{2}$

Substituting this into equation (42) above, where y = kR,

$$\frac{\mu V_0 R^2}{\hbar^2} \ll 1 \qquad (44)$$

The above inequality shows that if the potential is strong enough to bind a particle, the Born approximation then cannot be applied in the low energy limit.

The high energy limit - y large

$$\frac{\mu V_0}{2\hbar^2 k^2}\left[(cosy-1)^2+(siny-y)^2\right]^{\frac{1}{2}} \ll 1$$

In the first term; neglecting cosy for large y as compared to1, in the second termsiny can be maximally be 1 and hence can be neglected as compared to y, thus we have $(1+y^2)^{\frac{1}{2}} = y$, for $y \gg 1$

Thus, $\frac{\mu V_0}{2\hbar^2 k^2}[y] \ll 1, \frac{\mu V_0 kR}{\hbar^2 k^2} \ll 1\ ,\ \frac{\mu V_0 R}{\hbar^2 k} \ll 1$ (45)

This condition, equation (45), is generally satisfied at high energies for weak potentials.

5.0 Conclusion

Scattering by spherical square well potential is carried out using Born approximation and it's dependence on energy in the low and high limits has been calculated and examined.Results show that the scattering is isotropic (independent of scattering angle) at low energies and that the scattering shows a strong maximum in the forward direction (θ = 0) at high energies. The study has shown that Born approximation is only applicable in the high energy limit where the potential is weak. It indicates that the potential is strong enough to bind a particle.We have shown that if the scattering function has values much less than one,Born's approximation can safely be used in the high energy limit, because in the high energy limit the potential is too weak to bind a particle and it can be applied in the scattering at high energies. The dependence of scattering cross-section by spherical square well potential using Born's approximation can be applied in particle transport and nuclear cross-section calculations for gamma rays, electrons, positrons and neutrons[5,6,7].

For further studies, it is strongly recommended that Born's approximation be applied to scattering by infinite potential well problem; potential step or potential barriers; the harmonic oscillator problemand such other scattering potentials to check its further validity in those areas.

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