ON THE CONTRIBUTION OF HIGHER PARTIAL WAVES TO SCATTERING BY THE LONG–RANGE INVERSE POWER POTENTIALS

The Born approximation for phase shifts has been applied to estimate the contribution of higher partial waves to scattering by potentials vanishing asymptotically as \( r^{-n} \). Analytical expressions for corrections to a scattering amplitude, total and diffusion cross sections are given. The derived formulas can be used in a description of the electron, ion and atom collisions with atomic targets.

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1. THE BORN APPROXIMATION FOR PHASE SHIFTS

Let us consider a particle scattered by a central potential \( V(r) \). As it is well known, the scattering process is completely determined by the infinite set of phase shifts \( \delta_l \) produced by this potential and all the important quantities — the scattering amplitude, differential, total and momentum transfer (diffusion) cross sections may be expressed in terms of \( \delta_l \)'s. Thus the first step in scattering calculations is evaluation of the phase shifts. If the radial Schrödinger equation with the potential \( V(r) \) cannot be solved analytically for an arbitrary \( l \) (and usually it is so), we
must look for approximate, analytical or numerical, methods of evaluation of the phase shifts. For low angular momenta one usually solves numerically the radial Schrödinger equation while for higher partial waves the various approximate analytical methods are used [1, 2]. Among them one of the most widely used is the Born approximation.

We restrict ourselves to potentials with long-range tails of the form

\[ V(r) \simeq \frac{A}{r^n}. \]  

(1)

For potentials vanishing asymptotically faster than \( r^{-2} \) the Born approximation for the phase shifts has the form [1]

\[ \delta^B_l = - \frac{2mk}{\hbar^2} \int_0^\infty dr r^2 V(r) j_l^2(kr). \]  

(2)

For large \( l \) the particle will be mainly scattered by a tail of the potential. In such a case we may replace the potential \( V \) in Eq. (2) by its long-range part (1) and obtain

\[ \delta^B_l = - \frac{2mA}{\hbar^2} \int_0^\infty dr r^{-n+2} j_l^2(kr). \]  

(3)

For \( 2l + 3 > n \) the phase shift calculated using this expression is finite while for \( 2l + 3 \leq n \) the integral diverges in the lower limit. Using a relationship defining the spherical Bessel functions in terms of Bessel functions of half-integer order

\[ j_l(kr) = \sqrt{\frac{\pi}{2kr}} J_{l+\frac{1}{2}}(kr) \]  

(4)

the integral in Eq. (3) may be transformed to a form well known from the theory of Bessel functions and we obtain [2, 3]

\[ \delta^B_l = - \pi \left( \frac{mA}{\hbar^2} \right) \int_0^\infty dr r^{-n+1} J_{l+\frac{3}{2}}^2(kr) = \]

\[ = - \frac{\pi}{2} \left( \frac{mA}{\hbar^2} \right) \left( \frac{k}{2} \right)^{n-2} \frac{\Gamma(n-1)\Gamma(l+\frac{3}{2}-\frac{n}{2})}{\Gamma^2(\frac{n}{2})\Gamma(l+\frac{1}{2}+\frac{n}{2})} \]  

(5)

provided \( 2l + 3 > n \). We rewrite this expression in the form more convenient in further manipulations

\[ \delta^B_l = - \sqrt{\pi} \left( \frac{mA}{\hbar^2} \right) k^{n-2} \frac{\Gamma(\frac{3}{2}-\frac{n}{2})}{(n-1)\Gamma(\frac{n}{2})\Gamma(\frac{1}{2}+\frac{n}{2})} \] \( (a)_l \)

(6)

where \( (a)_l \) denotes the Pochhammer symbol

\[ (a)_l = \frac{\Gamma(a+l)}{\Gamma(a)}. \]  

(7)
We observe that although for \(2l + 3 < n\) the Born phase shift \(\delta_l^B\) does not exist, nevertheless we can define a quantity

\[
\tilde{\delta}_l^B = -\sqrt{\pi} \left( \frac{m^A}{\hbar^2} \right) k^{n-2} \frac{\Gamma \left( \frac{3}{2} - \frac{n}{2} \right)}{(n-1) \Gamma \left( \frac{n}{2} \right)} \frac{(\frac{3}{2} - \frac{n}{2})_l}{(\frac{1}{2} + \frac{n}{2})_l}, \tag{8}
\]

which is well defined for all \(l \geq 0\) provided \(n\) does not equal to an odd integer. This case would require a special treatment. However, such potentials are of less practical interest and we shall not consider them here.

2. EVALUATION OF SCATTERING AMPLITUDE AND CROSS SECTIONS

Let us assume that phase shifts for partial waves for which \(0 \leq l \leq l_0\) have been evaluated exactly by solving the radial Schrödinger equation and those for higher partial waves with \(l > l_0\) \((2l_0 + 5 > n)\) we have estimated using the Born approximation. Given the phase shifts we may approximate the scattering amplitude by an expression

\[
f(\theta) \simeq f_{l_0}(\theta) - \tilde{f}_{l_0}(\theta) + \tilde{f}^B(\theta), \tag{9}
\]

where

\[
f_{l_0}(\theta) = \frac{1}{2i k} \sum_{l=0}^{l_0} (2l + 1) (e^{2i \xi_l} - 1) P_l(\cos \theta), \tag{10}
\]

\[
\tilde{f}_{l_0}(\theta) = \frac{1}{k} \sum_{l=0}^{l_0} (2l + 1) \tilde{\delta}_l^B P_l(\cos \theta) \tag{11}
\]

and

\[
\tilde{f}^B(\theta) = \frac{1}{k} \sum_{l=0}^{\infty} (2l + 1) \tilde{\delta}_l^B P_l(\cos \theta). \tag{12}
\]

It must be pointed that \(\tilde{f}^B(\theta)\) defined by Eq. (12) is not the Born approximation to the scattering amplitude \(f(\theta)\). In principle, the amplitude \(\tilde{f}^B(\theta)\) may be calculated numerically to any desired accuracy retaining in the above sum sufficiently large number of terms. However, practically it would be difficult since for large \(l\) Legendre polynomials are rapidly oscillating functions of \(\theta\) and their numerical evaluation would be troublesome. An important property of the inverse power potentials is that, as we shall show below, \(\tilde{f}^B(\theta)\) may be written in a closed form. Substituting Eq. (8) into Eq. (12) we have

\[
\tilde{f}^B(\theta) = -\sqrt{\pi} \left( \frac{m^A}{\hbar^2} \right) k^{n-3} \frac{\Gamma \left( \frac{3}{2} - \frac{n}{2} \right)}{(n-1) \Gamma \left( \frac{n}{2} \right)} \sum_{l=0}^{\infty} (2l + 1) \frac{(\frac{3}{2} - \frac{n}{2})_l}{(\frac{1}{2} + \frac{n}{2})_l} P_l(\cos \theta). \tag{13}
\]
Using the formula (see Ref. [4], Eq. (5.10.1.17))
\[
\sum_{l=0}^{\infty} (2l+1) \frac{(2-a)_l}{(a)_l} P_l(x) = (a-1) \left( \frac{1-x}{2} \right)^{a-2}
\]  
(14)

with \( a = \frac{1}{2} + \frac{n}{2} \) we obtain
\[
f^B(\theta) = -\frac{\sqrt{\pi}}{2} \left( \frac{mA}{\hbar^2} \right) k^{n-3} \frac{\Gamma \left( \frac{3}{2} - \frac{n}{2} \right)}{\Gamma \left( \frac{n}{2} \right)} \sin^{n-3} \frac{\theta}{2}.
\]
(15)

Then substituting Eqs. (10), (11) and (15) to Eq. (9) we get the desired approximate expression for the scattering amplitude in which all sums have finite limits.

Similarly, the total cross section may be also written in a closed form. We start approximating the cross section by an expression
\[
Q_T \simeq Q_{T_{lo}} - \tilde{Q}_{T_{lo}} + \tilde{Q}_T^B
\]
(16)

where
\[
Q_{T_{lo}} = \frac{4\pi}{k^2} \sum_{l=0}^{l_0} (2l+1) \sin^2 \delta_l,
\]
(17)
\[
\tilde{Q}_{T_{lo}} = \frac{4\pi}{k^2} \sum_{l=0}^{l_0} (2l+1) \left( \delta_l^B \right)^2
\]
(18)

and
\[
\tilde{Q}_T^B = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left( \delta_l^B \right)^2.
\]
(19)

Obviously,
\[
\tilde{Q}_T^B = 2\pi \int_0^\pi d\theta \sin \theta \left| f^B(\theta) \right|^2.
\]
(20)

Substituting Eq. (15) and performing straightforward integration we obtain
\[
\tilde{Q}_T^B = \pi^2 \left( \frac{mA}{\hbar^2} \right)^2 k^{2n-6} \frac{\Gamma^2 \left( \frac{3}{2} - \frac{n}{2} \right)}{(n-2)\Gamma \left( \frac{n}{2} \right)}
\]
(21)

Substituting Eqs. (17), (18) and (21) to Eq. (16) we get the desired approximate closed expression for the total cross section.

Finally, we derive an expression for the diffusion cross section. We have
\[
Q_D \simeq Q_{D_{lo}} - \tilde{Q}_{D_{lo}} + \tilde{Q}_D^B.
\]
(22)
where

$$Q_{Dl_0} = \frac{4\pi}{k^2} \sum_{l=0}^{l_0-1} (l+1) \sin^2 (\delta_l - \delta_{l+1}) + \frac{4\pi}{k^2} (l_0 + 1) \sin^2 (\delta_{l_0} - \tilde{\delta}_{l_0+1})$$ \hspace{1cm} (23)

$$\tilde{Q}_{Dl_0}^B = \frac{4\pi}{k^2} \sum_{l=0}^{l_0} (l+1) \left( \tilde{\delta}_l^B - \tilde{\delta}_{l+1}^B \right)^2$$ \hspace{1cm} (24)

and

$$\tilde{Q}^B_D = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (l+1) \left( \tilde{\delta}_l^B - \tilde{\delta}_{l+1}^B \right)^2$$ \hspace{1cm} (25)

As

$$\tilde{Q}^B_D = 2\pi \int_0^\pi d\theta \sin \theta (1 - \cos \theta) \left| \tilde{f}^B(\theta) \right|^2,$$ \hspace{1cm} (26)

performing integration we get

$$\tilde{Q}^B_D = 2\pi^2 \left( \frac{mA}{\hbar^2} \right)^2 k^{2n-6} \frac{\Gamma^2(\frac{3}{2} - \frac{n}{2})}{(n-1)\Gamma^2(\frac{n}{2})}.$$ \hspace{1cm} (27)

3. DISCUSSION

In atomic physics two particular cases are interesting, namely $n = 4$ and $n = 6$. The former corresponds to the polarization interaction between a charged projectile and a neutral target while the latter corresponds to the Van der Waals interaction between neutrals. In both cases the coefficient $A$ is negative, i.e. $A = -|A|$, and Eqs. (8), (15), (21) and (27) take the form (for $n = 4$, $\tilde{f}^B(\theta)$ and $\tilde{Q}^B_T$ were given, in an implicit form, by Moiseiwitsch [5] and Thompson [6]):

for $n = 4$

$$\tilde{\delta}_l^B = 2\pi \left( \frac{|A|}{\hbar^2} \right)^2 \frac{k^2}{(2l-1)(2l+1)(2l+3)},$$ \hspace{1cm} (28)

$$\tilde{f}^B(\theta) = -\pi \left( \frac{|A|}{\hbar^2} \right) k \sin \frac{\theta}{2},$$ \hspace{1cm} (29)

$$\tilde{Q}^B_T = 2\pi^3 \left( \frac{|A|}{\hbar^2} \right)^2 k^2,$$ \hspace{1cm} (30)
\[ \tilde{Q}_B^D = \frac{8}{3} \pi^3 \left( \frac{m|A|}{\hbar^2} \right)^2 k^2, \]  
(31)

for \( n = 6 \)

\[ \delta_i^B = 6\pi \left( \frac{m|A|}{\hbar^2} \right)^2 \frac{k^4}{(2l-3)(2l-1)(2l+1)(2l+3)(2l+5)}; \]  
(32)

\[ \tilde{f}^B(\theta) = \frac{1}{3} \pi \left( \frac{m|A|}{\hbar^2} \right) k^3 \sin^3 \frac{\theta}{2}; \]  
(33)

\[ \tilde{Q}_T^B = \frac{1}{9} \pi^3 \left( \frac{m|A|}{\hbar^2} \right)^2 k^6, \]  
(34)

\[ \tilde{Q}_D^B = \frac{8}{45} \pi^3 \left( \frac{m|A|}{\hbar^2} \right)^2 k^6. \]  
(35)

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O METODZIE OSZACOWANIA WKLADU WYŻSZYCH FAL CZĄSTKOWYCH DO ROZPRASZANIA NA POTENCJALACH DŁUGOZASIĘGOWYCH

W oparciu o przybliżenie Borna oszacowano wkład wyższych fal cząstkowych do rozpraszania na potencjalach zanikających asymptotycznie jak $r^{-n}$. Podano analityczne wyrażenia na poprawki do amplitudy rozpraszania oraz całkowitego i dyfuzyjnego przekroju czynnego. Otrzymane wzory znajdują zastosowanie przy opisie zderzeń elektronów, jonów i atomów z atomami.

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