Phase shift analysis

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Two methods for treating scattering problems are discussed: the Born approximation and the method of partial waves. The Born approximation is most applicable when the kinetic energy of the incoming beam is large compared with the scattering potential, whereas the method of partial waves is most readily applied when the energy of the incoming particles is low. The two methods thus tend to complement each other. The relation of virtual levels to the resonant scattering of appropriate partial waves is discussed here.

Ramsauer-Townsend effect and Frank-Hertz experiment
Levinston's theorem
S matrix element
Effective potential range
Scattering length
Breit-Wigner formula

1. Scattering by potential

The scattered wave function has the general form;

$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = a_l[\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)],$$

except at the origin, in the case when the potential energy is zero. Since $n_l(kr)$ diverges at the origin, the wave function has the form

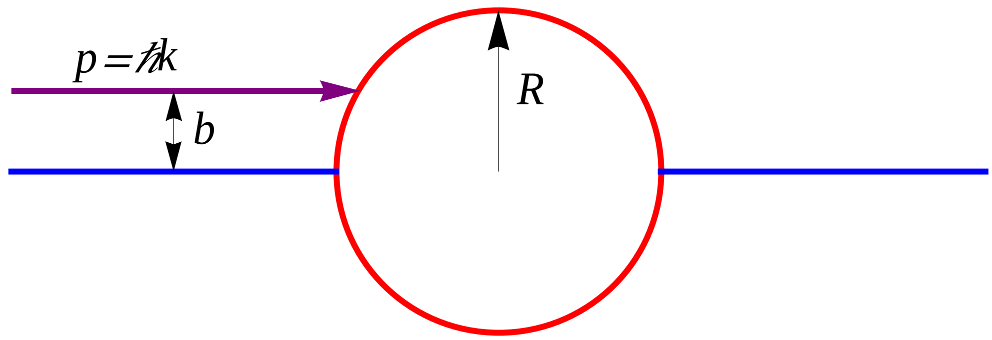
$$R_{kl}(r) = \frac{u_{kl}(r)}{r} = d_l j_l(kr),$$

in the vicinity of the origin. We need to determine the phase shift from appropriate boundary conditions; the continuity of the wave function and the derivative of the wave function.

((Classical theory))

The angular momentum is conserved; $l = kb$, where b is the impact parameter and k is the wave number of the incident particle. The scattering occurs when b is lower than the radius of the target; $b<R$. Then we have

$$l = kb < kR = l_{\max}$$



When energy is low such that $kR << 1$, l_{max} is small is equal to zer0, S wave). Partial waves for higher l are, in general, unimportant.

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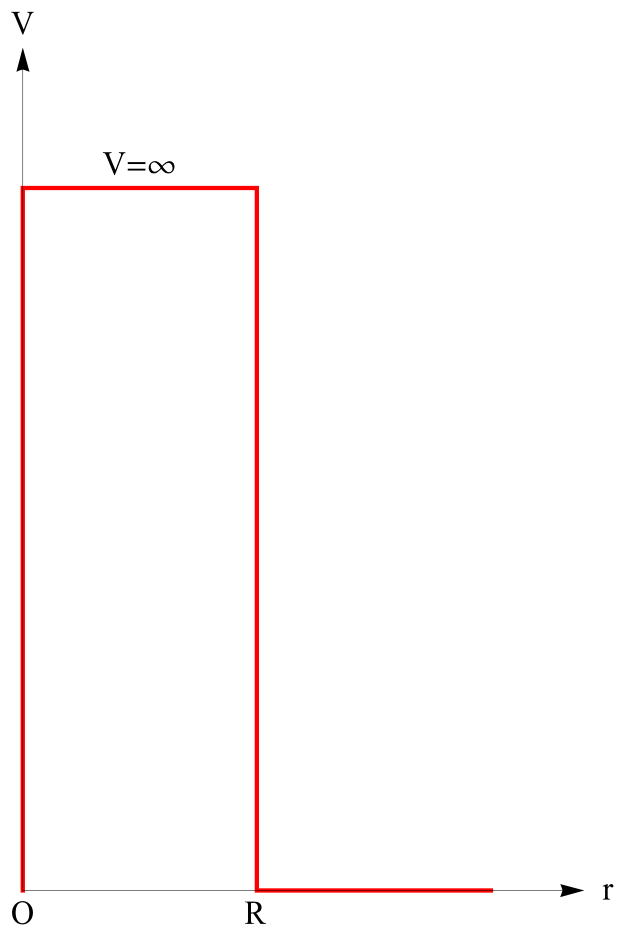
2. Hard sphere scattering (I)

We consider the scattering from the repulsive potential

$$V(r) = \begin{cases} \infty & r < R \\ 0 & r > R \end{cases}$$



The wave function is given by

$$R_{kl}(r) = e^{i\delta_l}[\cos\delta_l\, j_l(kr) - \sin\delta_l n_l(kr)]\,.$$

for $r>R$. The wave function must vanish at $r = R$ because the sphere is impenetrable.

$$R_{kl}(r)|_{r=R} = 0 = e^{i\delta_l}[\cos\delta_l\, j_l(kR) - \sin\delta_l n_l(kR)]\,,$$

or

$$\tan\delta_l = \frac{j_l(kR)}{n_l(kR)}\,.$$

Thus the phase shifts are known for any *l*. The values of δ_l in the limit of $kR<<1$ are as follows for each *l*.

((**Mathematica**)) Series expansion of $f_l(\rho) = \dfrac{j_l(\rho)}{n_l(\rho)}$ around $\rho = 0$

```
Clear["Global`*"];
f1[L1_, z1_] :=
 Series[SphericalBesselJ[L1, z1] / SphericalBesselY[L1, z1], {z1, 0, 12}] // Normal;
Prepend[Table[{L, f1[L, z]}, {L, 0, 4}],
  {"L", " f[L,z]"}] // TableForm
```

L	f[L,z]
0	$-z-\frac{z^3}{3}-\frac{2z^5}{15}-\frac{17z^7}{315}-\frac{62z^9}{2835}-\frac{1382z^{11}}{155925}$
1	$-\frac{z^3}{3}+\frac{z^5}{5}-\frac{z^7}{7}+\frac{8z^9}{81}-\frac{34z^{11}}{495}$
2	$-\frac{z^5}{45}+\frac{z^7}{189}-\frac{z^{11}}{2673}$
3	$-\frac{z^7}{1575}+\frac{z^9}{10125}-\frac{z^{11}}{185625}$
4	$-\frac{z^9}{99225}+\frac{z^{11}}{848925}$

Let us now consider the low energy limit ($kR << 1$)

For $\rho = kR << 1$

$$j_l(\rho) \to \frac{\rho^l}{(2l+1)!!} \qquad (\rho \to 0)$$

$$n_l(\rho) \to -\frac{(2l-1)!!}{\rho^{l+1}}, \qquad (\rho \to 0)$$

where

$$(2l+1)!! = 1\cdot 3\cdot 5\cdot 7\cdot 9\cdots(2l-1)(2l+1).$$

Then we have

$$\tan\delta_l = \frac{j_l(\rho)}{n_l(\rho)} = -\frac{\rho^{2l+1}}{(2l+1)!!}\frac{1}{(2l-1)!!} \to 0,$$

or

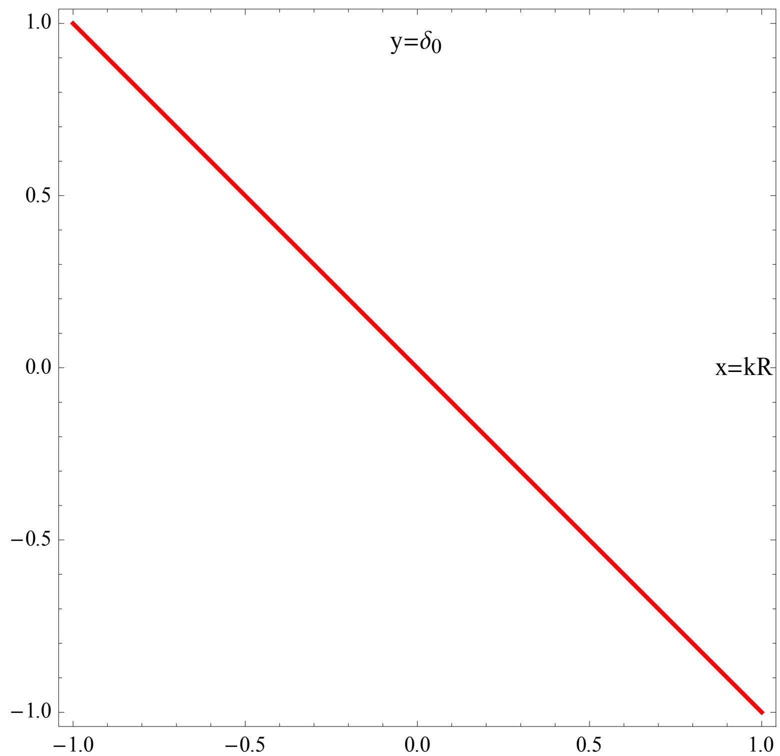
$$\delta_l = 0 \text{ for any } l \qquad (\text{in the limit of } \rho \to 0).$$

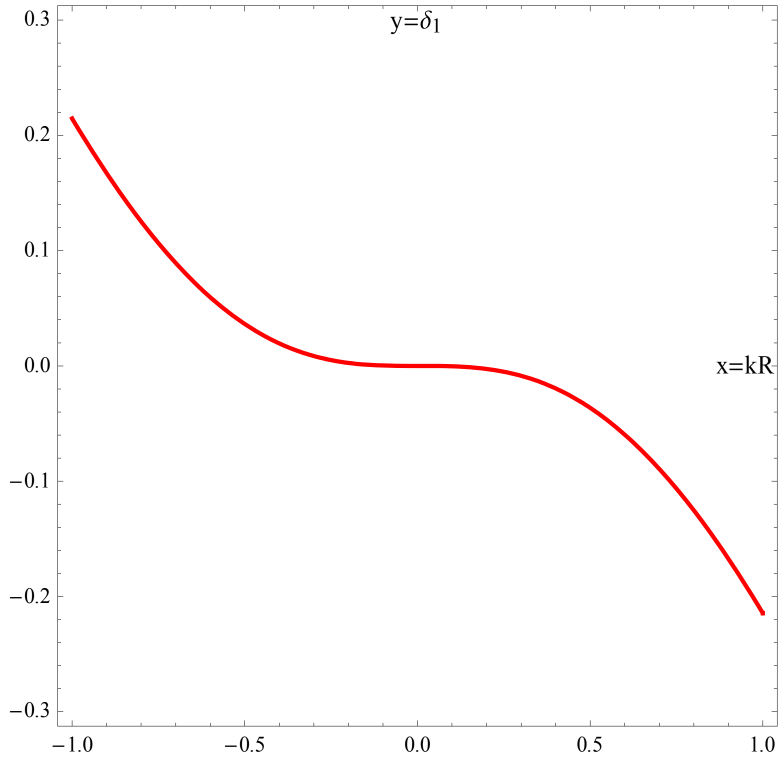
((**Note**))

$$\tan\delta_0 = \delta_0 = -\rho\,,$$

$$\tan\delta_1 = \delta_1 = -\frac{\rho^3}{3}\,,$$

$$\tan\delta_2 = \delta_2 = -\frac{\rho^5}{45}$$





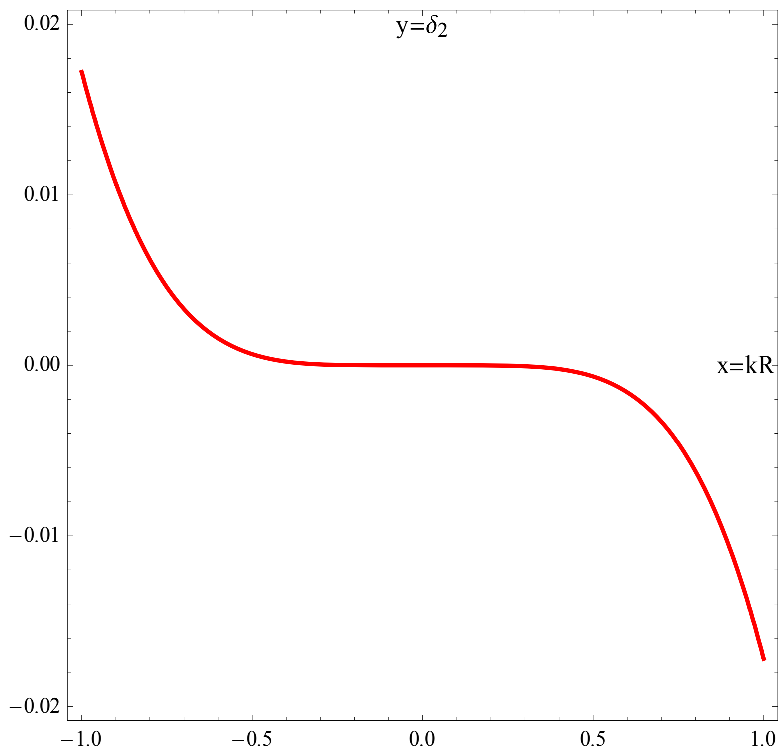


Fig. ContourPlot of the phase shift δ_l vs $x = kR$ for $l = 0$, 1, and 2.

3. Hard sphere scattering (II): Low energy case (kR<<1)

We consider the $l = 0$ case (S-wave scattering).
For $l = 0$,

$$\tan\delta_0 = \frac{j_0(kR)}{n_0(kR)} = -\tan(kR)$$

or

$$\delta_0 = -kR \qquad (\delta_0 < 0).$$

Then we have

$$\begin{aligned} R_{k,l=0}(r) &= e^{i\delta_0}[\cos\delta_0 j_0(kr) - \sin\delta_0 n_0(kr)] \\ &= \frac{e^{i\delta_0}}{kr}[\cos\delta_0 \sin_0(kr) + \sin\delta_0 \cos_0(kr)] \\ &= \frac{e^{i\delta_0}}{kr}\sin(kr + \delta_0) \end{aligned}$$

where

$$j_0(x) = \frac{\sin x}{x},$$

$$n_0(x) = -\frac{\cos x}{x}.$$

Since $\delta_0 = -kR$, we have

$$R_{k,l=0}(r) = \frac{e^{i\delta_0}}{kr}\sin[k(r-R)]$$

Then we have

$$\sigma_{tot} = \frac{4\pi}{k^2}\sin^2\delta_0 \approx \frac{4\pi}{k^2}k^2R^2 = 4\pi R^2,$$

which is four times the geometric cross section πR^2. *In this case* σ_{tot} *is the total surface area of the sphere with a radius R. The waves feel their way around the whole sphere.*

((**Note-1**))

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \ .$$

((Note-2)) Direct calculation of differential equation

Here we derive the above solution directly from solving the differential equation.

$$u''(r) + [k^2 - U(r) - \frac{l(l+1)}{r^2}]u(r) = 0 , \qquad (1)$$

where

$$u(r) = rR(r) .$$

When $l = 0$ and $U(r) = 0$, we get the differential equation

$$u''(r) + k^2 u(r) = 0 ,$$

$$u = rR(r) = C\sin(kr + \delta_0)$$

For $r = R$,

$$u(r) = 0,$$

or

$$kR = -\delta_0 .$$

4. Hard sphere scattering (III): High energy case ($kR >> 1$)

We consider the semi-classical situation where $kR >> 1$

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_{l=0}^{l=kR}(2l+1)\sin^2\delta_l \qquad (1)$$

with

$$\sin^2\delta_l = \frac{\tan^2\delta_l}{1+\tan^2\delta_l} = \frac{\{j_l(kR)\}^2}{\{j_l(kR)\}^2 + \{n_l(kR)\}^2}$$

with

$$\tan\delta_l = \frac{j_l(kR)}{n_l(kR)}$$

The asymptotic form is given by

$$j_l(kR) \approx \frac{1}{kR}\sin(kR - \frac{l\pi}{2}),$$

$$n_l(kR) \approx -\frac{1}{kR}\cos(kR - \frac{l\pi}{2}),$$

for $kR >> 1$. Then we have

$$\sin^2\delta_l = \sin^2(kR - \frac{l\pi}{2}), \qquad (\delta_l = -kR + \frac{l\pi}{2})$$

We also have

$$\sin^2\delta_{l+1} = \sin^2(kR - \frac{(l+1)\pi}{2}) = \cos^2(kR - \frac{l\pi}{2}).$$

For an adjacent pair of partial waves

$$\sin^2\delta_l + \sin^2\delta_{l+1} = \sin^2(kR - \frac{l\pi}{2}) + \cos^2(kR - \frac{l\pi}{2}) = 1.$$

With so many *l*-values contributing to Eq.(1),

$$\langle \sin^2\delta_l \rangle \approx \frac{1}{2},$$

and

$$\begin{aligned}\sigma_{tot} &\approx \frac{4\pi}{k^2}\sum_{l=0}^{l=kR}(2l+1)\langle \sin^2\delta_l \rangle \\ &= \frac{2\pi}{k^2}\sum_{l=0}^{l=kR}(2l+1) \\ &= \frac{2\pi}{k^2}(kR+1)^2 \approx 2\pi R^2\end{aligned},$$

which is twice larger than the geometric cross section πR^2.

5. Origin of $\sigma_{tot} \approx 2\pi R^2$ for kR>>1 (Sakurai and Napolitano)

The scattering amplitude is given by

$$
\begin{aligned}
f(\theta) &= f_{reflection} + f_{shadow} \\
&= \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta) \\
&= \frac{1}{2ik}\sum_{l=0}^{kR}(2l+1)[e^{2i\delta_l}-1]P_l(\cos\theta) \\
&= \frac{1}{2ik}\sum_{l=0}^{kR}(2l+1)e^{2i\delta_l}P_l(\cos\theta) + \frac{i}{2k}\sum_{l=0}^{kR}(2l+1)P_l(\cos\theta)
\end{aligned}
$$

where

$$
f_{reflection} = \frac{1}{2ik}\sum_{l=0}^{kR}(2l+1)e^{2i\delta_l}P_l(\cos\theta),
$$

$$
f_{shadow} = \frac{i}{2k}\sum_{l=0}^{kR}(2l+1)P_l(\cos\theta).
$$

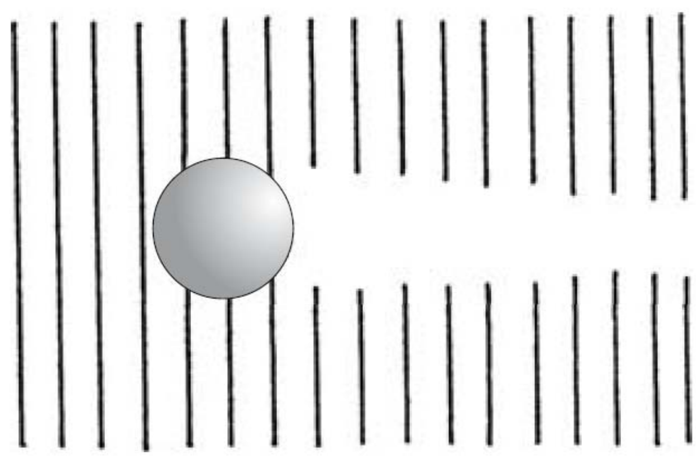


Fig. Shadow scattering (**Schwabl**).

Now we calculate the contribution from the reflection,

$$\begin{aligned}\int d\Omega \left| f_{reflection} \right|^2 &= \frac{2\pi}{4k^2}\sum_{l=0}^{kR}\sum_{l'=0}^{kR}(2l+1)(2l'+1)e^{-2i\delta_l+2i\delta_{l'}}\int_{-1}^{1} d(\cos\theta)P_l(\cos\theta)P_{l'}(\cos\theta) \\ &= \frac{2\pi}{4k^2}\sum_{l=0}^{kR}\sum_{l'=0}^{kR}(2l+1)(2l'+1)e^{-2i\delta_l+2i\delta_{l'}}\,\frac{2}{2l+1}\delta_{l,l'} \\ &= \frac{\pi}{k^2}\sum_{l=0}^{kR}(2l+1) \\ &\approx \frac{\pi}{k^2}k^2R^2 = \pi R^2\end{aligned}$$

where

$$\int \sin\theta d\theta P_l(\cos\theta)P_{l'}(\cos\theta) = \frac{2}{2l+1}\delta_{l,l'}$$

It is particularly strong in the forward direction because $P_l(\cos\theta) = 1$ for θ = 0, and the contribution from various *l*-values and add up coherently. The contribution from the shadow is obtained as

$$\begin{aligned}\int d\Omega \left| f_{shadow} \right|^2 &= \frac{2\pi}{4k^2}\sum_{l=0}^{kR}(2l+1)^2\int_{-1}^{1} d(\cos\theta)[P_l(\cos\theta)]^2 \\ &= \frac{\pi}{k^2}\sum_{l=0}^{kR}(2l+1) = \pi R^2\end{aligned}$$

Note that

$$\int d\Omega \left| f_{reflection} + f_{shadow} \right|^2 = \int d\Omega (\left| f_{reflection} \right| + \left| f_{shadow} \right|^2 + 2\,\mathrm{Re}[f_{shadow}{}^* f_{reflection}])$$

The interference between f_{shadow} and $f_{reflection}$ vanishes:

$$\int d\Omega\, \mathrm{Re}[f_{shadow}{}^* f_{reflection}] = 0$$

The reason for this is as follows. We note that

$$\delta_l = -kR + \frac{l\pi}{2},$$

and

$$\delta_0 = -kR\,.$$

for kR>>1. Then we have

$$
\begin{aligned}
f_{reflection} &= \frac{1}{2ik}\sum_{l=0}^{kR}(2l+1)e^{2i\delta_l}P_l(\cos\theta) \\
&= \frac{1}{2ik}e^{2i\delta_0}\sum_{l=0}^{kR}(2l+1)(-1)^l P_l(\cos\theta)
\end{aligned}
$$

since $e^{il\pi} = (-1)^l$. Then we get

$$
\begin{aligned}
\mathrm{Re}[f_{shadow}{}^* f_{reflection}] &= \mathrm{Re}[\frac{-i}{2k}\sum_{l=0}^{kR}(2l+1)P_l(\cos\theta)\frac{1}{2ik}e^{2i\delta_0}\sum_{l'=0}^{kR}(2l'+1)(-1)^l P_{l'}(\cos\theta) \\
&= \mathrm{Re}[-\frac{1}{4k^2}e^{2i\delta_0}\sum_{l=0}^{kR}\sum_{l'=0}^{kR}(-1)^l(2l+1)(2l'+1)P_l(\cos\theta)P_{l'}(\cos\theta)]
\end{aligned}
$$

So we have the interference between f_{shadow} and $f_{reflection}$ as

$$
\begin{aligned}
I_{sr} &= \int d\Omega\,\mathrm{Re}[f_{shadow}{}^* f_{reflection}] \\
&= \mathrm{Re}[-\frac{1}{4k^2}e^{2i\delta_0}\sum_{l=0}^{kR}\sum_{l'=0}^{kR}(-1)^l(2l+1)(2l'+1)\int d\Omega P_l(\cos\theta)P_{l'}(\cos\theta)] \\
&= \mathrm{Re}[-\frac{1}{4k^2}e^{2i\delta_0}\sum_{l=0}^{kR}\sum_{l'=0}^{kR}(-1)^l(2l+1)(2l'+1)\frac{4\pi\delta_{l,l'}}{2l+1}] \\
&= \mathrm{Re}[-\frac{\pi}{k^2}e^{2i\delta_0}\sum_{l=0}^{kR}(-1)^l(2l+1)] \\
&= \mathrm{Re}[-\frac{\pi}{k^2}e^{2i\delta_0}(-1)^{kR}(1+kR)] \\
&= \mathrm{Re}[-\frac{\pi}{k^2}e^{-2ikR}(-1)^{kR}(1+kR)] \\
&\approx -\frac{\pi R^2}{kR}(-1)^{kR}\cos(2kR)
\end{aligned}
$$

or

$$
\frac{I_{sr}}{\pi R^2} = (-1)^{kR+1}\frac{\cos(2kR)}{kR},
$$

where we assume that kR is integer. We also use the formula

$$
\sum_{l=0}^{kR}(-1)^l(2l+1) = (-1)^{kR}(1+kR).
$$

We make a plot of I_{sr} as a function of kR (=integer). We find that I_{sr} oscillates with kR and reduces to zero for sufficiently large kR.

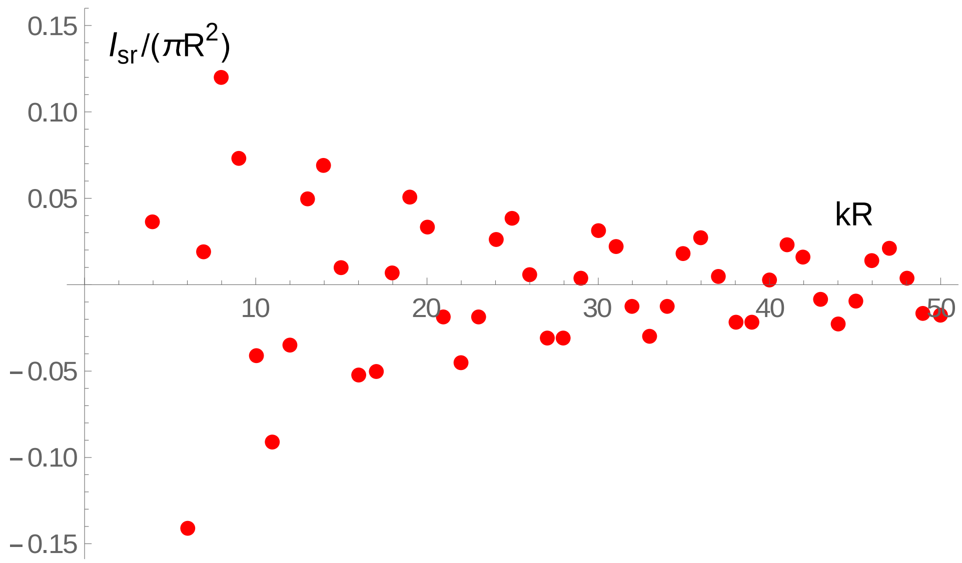


Fig. Plot of $I_{sr}/(\pi R^2)$ as a function of kR (= integer).

6. Optical theorem and shadow part

The shadow is due to the destructive interference between the incident wave and the newly scattered wave. We now calculate

$$\begin{aligned}\frac{4\pi}{k}\mathrm{Im}[f_{shadow}(\theta)] &\approx \frac{4\pi}{k}\mathrm{Im}[f_{shadow}(\theta=0)] \\ &= \frac{2\pi}{k^2}\sum_{l=0}^{kR}(2l+1)P_l(1) \\ &= \frac{2\pi}{k^2}\sum_{l=0}^{kR}(2l+1) \\ &= \frac{2\pi}{k^2}(kR+1)^2 \\ &\approx 2\pi R^2\end{aligned}$$

where

$$P_l(1) = 1$$

Thus we have the optical theorem;

$$\sigma_{tot} = \frac{4\pi}{k}\mathrm{Im}[f(\theta=0)] \approx \frac{4\pi}{k}\mathrm{Im}[f_{shadow}(\theta=0)]$$

since $\sigma_{tot} \approx 2\pi R^2$.

7. Physical meaning (D. Bohm, Quantum Theory)

The total cross section is given by

(i) Quantum limit

The quantum scattering occurs when $kR << 1$ ($\lambda >> 2\pi R$)

$$\sigma_T = 4\pi R^2. \qquad \text{(long-wavelength)}$$

As the wavelength goes below the size of the sphere, the first effect will be to introduce waves of higher angular momentum. So that the cross section becomes angular dependent. As the wavelength made still shorter, however, and the classical region is approached, the cross section once again becomes spherically symmetrical, with a value reduced to pR2, except for a region near $\theta = 0$ with an angular width of the order of

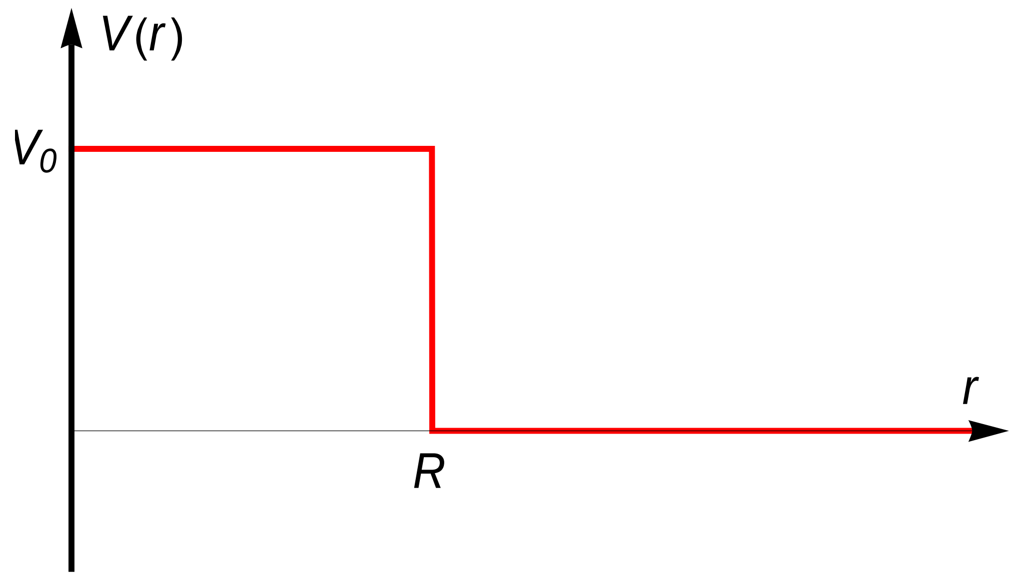
$$\Delta\theta \approx \frac{\lambda}{2\pi R}.$$

The large projection in the forward direction is essentially a diffraction effect, containing a total cross section of πR^2. Thus, for very short wavelengths, the total cross section is $2\pi R^2$.

(ii) Classical limit

$$\sigma_T = \pi R^2.$$

8. Finite repulsive potential



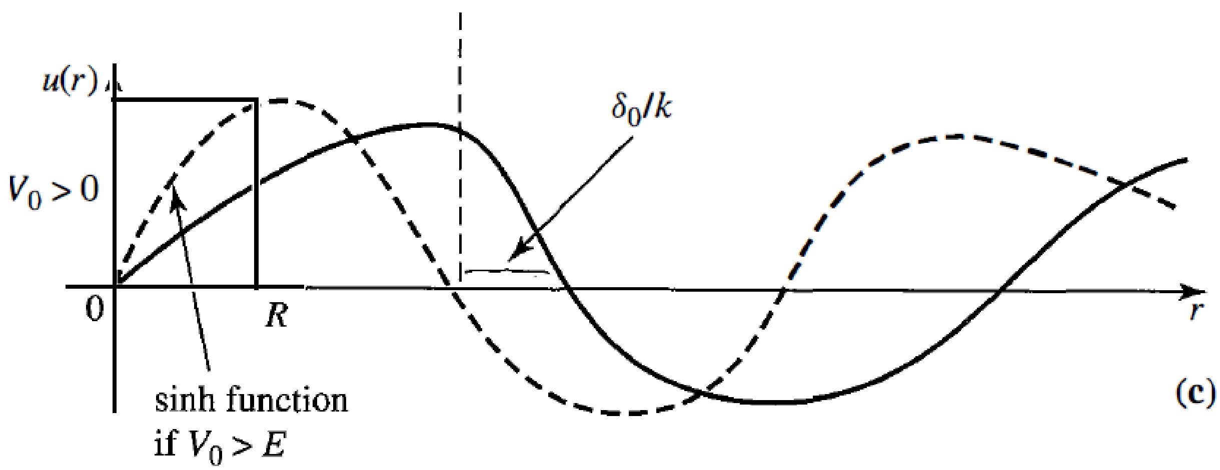


Fig. Plot of $u(r)$ as a function of r. (**Sakurai**). $R_{out}(r) = \frac{C}{r}\sin(kr + \delta_0)$ for $r>R$, with $\delta_0 < 0$.

For $l = 0$ (S-wave)

$$u''(r) + [k^2 - U(r)]u(r) = 0\,, \qquad (1)$$

where

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

and

$$u(r) = rR(r).$$

For $r<R$, we have

$$u''(r) - (-k^2 + k_0^{\;2})u(r) = 0,$$

where

$$U_0 = \frac{2\mu}{\hbar^2}V_0 = k_0^{\;2} > k^2.$$

and

$$\kappa = \sqrt{k_0^{\;2} - k^2}$$

Noting the boundary condition: $u = 0$ at r=0, the inside solution $u(r)$ can be obtained as

$$u_{in}(r) = A\sinh(\kappa r),$$

For $r>R$

$$u''(r) + k^2 u(r) = 0,$$

$$u_{out}(r) = C\sin(kr + \delta_0),$$

or

$$R_{out}(r) = \frac{C}{r}\sin(kr + \delta_0).$$

((**Boundary condition**))

We make sure that u is continuous and has a constant first derivative at $r = R$. The wave function and its derivative are continuous at $r = R$;

$$C\sin(kR + \delta_0) = A\sinh(\kappa R)$$

$$Ck\cos(kR + \delta_0) = A\kappa\cosh(\kappa R)$$

Then we get

$$\tan(kR + \delta_0) = \frac{k}{\kappa}\tanh(\kappa R) = \frac{kR}{\kappa R}\tanh(\kappa R)$$

with

$$\frac{kR}{\kappa R} = \sqrt{\frac{k^2R^2}{U_0R^2 - k^2R^2}} = \sqrt{\frac{k^2}{k_0^{\,2} - k^2}}\,.$$

For kR<<1, we have

$$kR + \delta_0 \approx \frac{kR}{\kappa R}\tanh(\kappa R)\,.$$

The total cross section is given by

$$\sigma_{tot} = \frac{4\pi}{k^2}\sin^2\delta_0 \approx \frac{4\pi}{k^2}\delta_0^{\,2} = 4\pi R^2[\frac{\tanh(\kappa R)}{\kappa R} - 1]^2.$$

For kR<<1, we have

$$\frac{\tanh(\kappa R)}{\kappa R} - 1 \approx \frac{1}{3}(\kappa R)^2\,.$$

$$\delta_0 \approx kR[\frac{\tanh(\kappa R)}{\kappa R} - 1] = kR\frac{1}{3}(k_0R)^2 > 0.$$

Then we get the total cross section as

$$\sigma_{tot} = \frac{4}{9}\pi k_0^{\,4}R^6 = \frac{16\pi\mu^2V_0^{\,2}}{9\hbar^4}R^6.$$

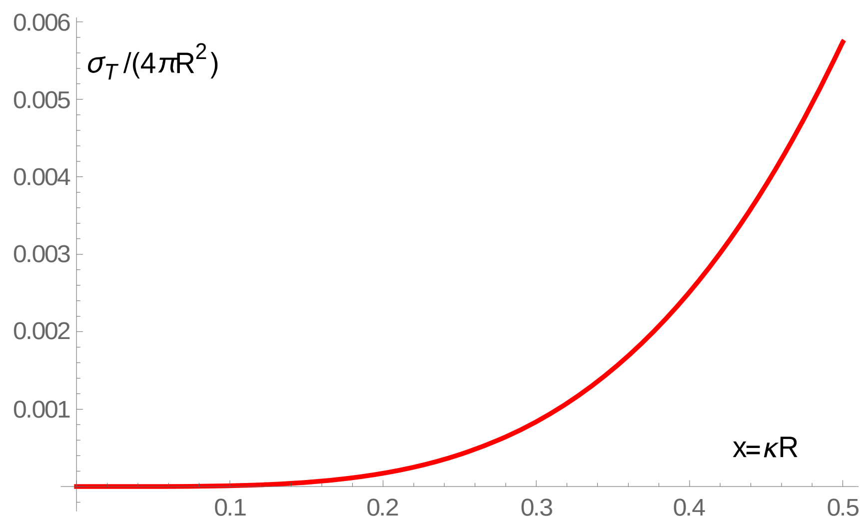


Fig. $y = \sigma_{tot} / (4\pi R^2)$ vs $x = \kappa R$.

9. Attractive Square-well potential: low- energy scattering

We consider the spherical square-well potential in three dimensions given by

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

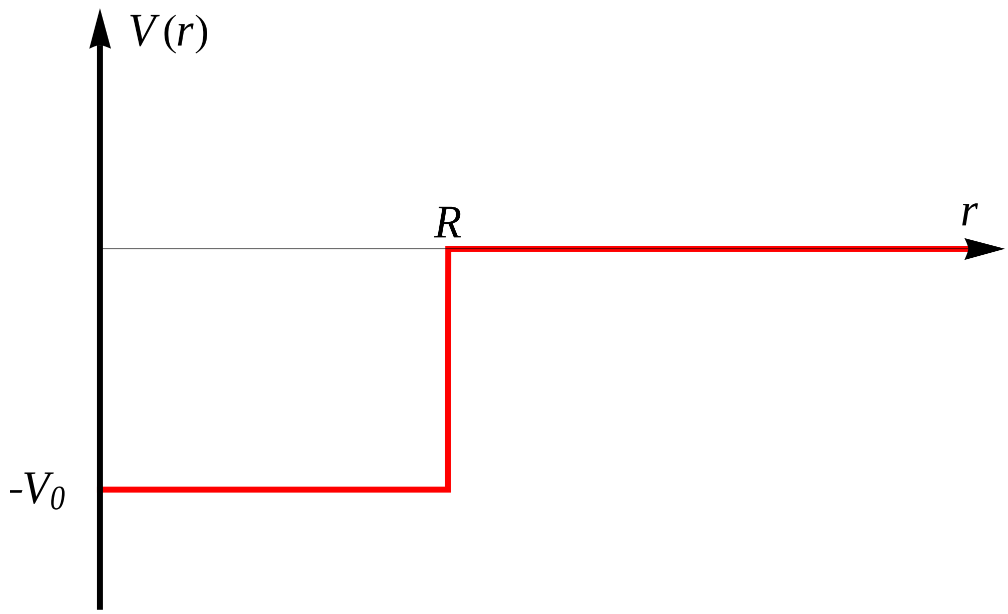


Fig. Attractive potential.

For $l = 0$ (S-wave)

$$u''(r) + [k^2 - U(r)]u(r) = 0, \tag{1}$$

where

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

$$E = \frac{\hbar^2}{2\mu} k^2,$$

and

$$u(r) = rR(r).$$

For $r<R$, we have

$$u''(r) + (k^2 + U_0)u(r) = 0,$$

where

$$U_0 = \frac{2\mu}{\hbar^2}V_0 = k_0^{\ 2}.$$

Noting the boundary condition: $u = 0$ at r=0, the inside solution $u(r)$ can be obtained as

$$u_{in}(r) = A\sin(\kappa_s r),$$

where A is an arbitrary constant,

$$\kappa_s = \sqrt{k^2 + U_0} = \sqrt{k^2 + k_0^{\ 2}}.$$

For $r>R$

$$u''(r) + k^2 u(r) = 0,$$

$$u_{out}(r) = C\sin(kr + \delta_0),$$

or

$$R_{out}(r) = \frac{C}{r}\sin(kr + \delta_0).$$

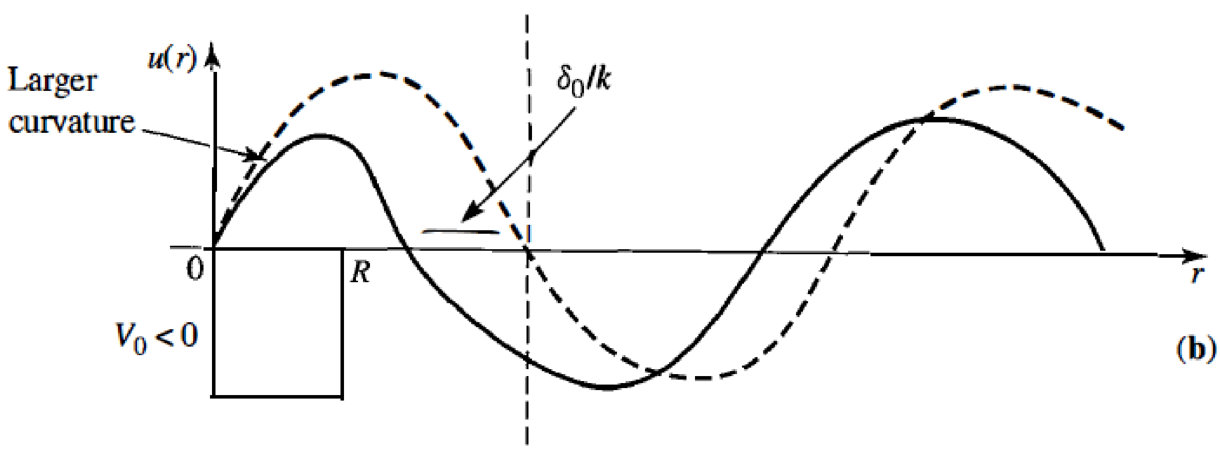


Fig. Plot of $u(r)$ as a function of r. (**Sakurai**). $u(r) = \frac{C}{r}\sin(kr + \delta_0)$ for $r>R$, with $\delta_0 > 0$.

((**Boundary condition**))

We make sure that u is continuous and has a constant first derivative at $r = R$. The wave function and its derivative are continuous at $r = R$;

$$C\sin(kR+\delta_0) = A\sin(\kappa_s R)\,,$$

$$Ck\cos(kR+\delta_0) = A\kappa_s\cos(\kappa_s R)\,,$$

Then we get

$$\tan(kR+\delta_0) = \frac{k}{\kappa_s}\tan(\kappa_s R) = \frac{kR}{\kappa_s R}\tan(\kappa_s R)$$

or

$$\frac{\tan(kR)+\tan\delta_0}{1-\tan\delta_0\tan(kR)} = \frac{kR}{\kappa_s R}\tan(\kappa_s R)$$

or

$$\tan\delta_0 = \frac{\dfrac{kR}{\kappa_s R}\tan(\kappa_s R)-\tan(kR)}{1+\dfrac{kR}{\kappa_s R}\tan(\kappa_s R)\tan(kR)}$$

with

$$\frac{kR}{\kappa_s R} = \sqrt{\frac{k^2R^2}{k^2R^2+U_0R^2}} = \sqrt{\frac{k^2}{k^2+k_0{}^2}}$$

((**Note**))

$$\begin{aligned}R_{out}(r) &= e^{i\delta_0}[\cos\delta_0 j_0(kr)-\sin\delta_0 n_0(kr)]\\ &= e^{i\delta_0}[\cos\delta_0\frac{\sin(kr)}{kr}+\sin\delta_0\frac{\cos(kr)}{kr}]\\ &= e^{i\delta_0}\frac{\sin(kr+\delta_0)}{kr}\\ &= C\frac{1}{r}\sin(kr+\delta_0)\end{aligned}$$

10. Total cross section for the attractive square-well potential: exact calculation

Here we discuss the exact expression for the total cross section for the S-wave scattering.

(a) The total cross section σ_{tot}

Here we start with the expression for $\tan\delta_0$ for the S wave, which is given by

$$\tan\delta_0 = \frac{\frac{kR}{\kappa_s R}\tan(\kappa_s R) - \tan(kR)}{1 + \frac{kR}{\kappa_s R}\tan(\kappa_s R)\tan(kR)}. \qquad \text{(exact expression)} \tag{1}$$

The total cross section can be obtained as

$$\begin{aligned}
\sigma_{tot} &= \frac{4\pi}{k^2}\sin^2\delta_0 \\
&= \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0} \\
&= \frac{4\pi}{k^2}\frac{1}{1+\dfrac{\left(1+\frac{kR}{\kappa R}\tan(\kappa_s R)\tan(kR)\right)^2}{\left(\frac{kR}{\kappa R}\tan(\kappa_s R)-\tan(kR)\right)^2}} \\
&= \frac{4\pi}{k^2}\frac{\left(\frac{kR}{\kappa_s R}\tan(\kappa_s R)-\tan(kR)\right)^2}{\left(\frac{kR}{\kappa_s R}\tan(\kappa_s R)-\tan(kR)\right)^2+\left(1+\frac{kR}{\kappa_s R}\tan(\kappa_s R)\tan(kR)\right)^2} \qquad (2) \\
&= 4\pi R^2\cos^2(kR)\frac{\left(\frac{\tan(\kappa_s R)}{\kappa_s R}-\frac{\tan(kR)}{kR}\right)^2}{[1+\left(\frac{kR}{\kappa_s R}\right)^2\tan(\kappa_s R)^2]}
\end{aligned}$$

For $kR \ll 1$, we get

$$\begin{aligned}
\sigma_{tot} &\approx 4\pi R^2\left(\frac{\tan(\kappa_s R)}{\kappa_s R}-\frac{\tan(kR)}{kR}\right)^2 \\
&\approx 4\pi R^2\left(\frac{\tan(\kappa_s R)}{\kappa_s R}-1\right)^2
\end{aligned} \tag{3}$$

σ_{tot} becomes zero when

$$\frac{\tan(\kappa_s R)}{\kappa_s R} = 1, \qquad (4)$$

or

$\kappa_s R = 4.49341$ (1.430 π), 7.72525 (2.459 π), 10.9041 (= 3.471 π), 14.0662 (= 4.477 π).

When $\tan(\kappa_s R) = \infty$ ($\kappa_s R = \pi/2, 3\pi/2, 5\pi/2, \ldots$),

$$\sigma_{tot} = \frac{4\pi}{k^2},$$

which becomes infinity as $k \to 0$.

(b) Phase shift δ_0

We start with another expression of

$$\tan(kR + \delta_0) = \frac{\tan(kR) + \tan\delta_0}{1 - \tan(kR)\tan\delta_0} = \frac{kR}{\kappa_s R}\tan(\kappa_s R). \qquad \text{(exact expression)}$$

As long as $\tan(\kappa_s R)$ is not too large, $\frac{kR}{\kappa_s R}\tan(\kappa_s R) << 1$. Then we have

$$\tan(kR + \delta_0) \approx kR + \delta_0 = \frac{kR}{\kappa_s R}\tan(\kappa_s R)$$

or

$$\delta_0 = kR[\frac{\tan(\kappa_s R)}{\kappa_s R} - 1].$$

Using this value of δ_0, the total cross section is obtained as

$$\sigma_{tot} = \frac{4\pi}{k^2}\sum_{l=0}^{l_{\max}}(2l+1)\sin^2\delta_l$$
$$\approx \frac{4\pi}{k^2}\sin^2\delta_0$$
$$= \frac{4\pi}{k^2}k^2R^2[\frac{\tan(\kappa_s R)}{\kappa_s R}-1]^2 \qquad (5)$$
$$= 4\pi R^2[\frac{\tan(\kappa_s R)}{\kappa_s R}-1]^2$$

which is the same as Eq.(4). We make a plot of this σ_{tot} as a function of $\kappa_s R$. This function becomes zero at $\kappa_s R$ = 4.49341 and 7.72525, 10.9041, 14.0662,…(Ramsauer effect) and becomes infinity at $\kappa_s R$ = π/2, 3π/2,…. (resonance).

We note that the attractive scattering becomes transparent to the incident beam at

$$\frac{\tan(\kappa_s R)}{\kappa_s R} = 1.$$

Such resonant transparency of an attractive well is experimentally observed in the scattering of low energy electrons by rare gas atoms. The vanishing of the scattering cross-section at a certain low values of the energy is found in a number of wave processes. For example, He or other noble gas atoms are practically transparent to slow electrons of about 0.7 eV energy, while smokes consisting of particles homogeneous in size are virtually transparent to light in a narrow wavelength region.

(c) **Numerical calculation**

We make a plot of $\sigma_{tot}/(4\pi R^2)$ as a function of $x = \kappa_s R$. This function becomes zero at $\kappa_s R$ = 4.49341 and 7.72525, and becomes infinity at $\kappa_s R$ = π/2, 3π/2,….

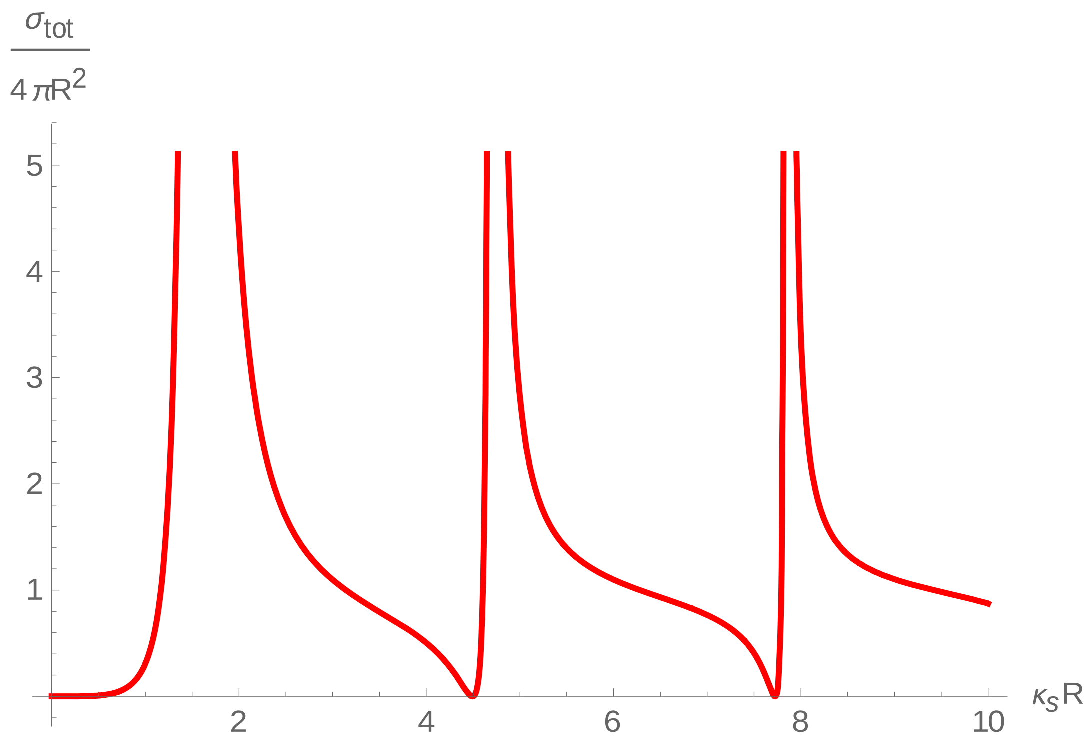


Fig. Plot of $[\frac{\tan(\kappa_s R)}{\kappa_s R} - 1]^2$ as a function of $\kappa_s R$.

11. Ramsauer-Townsend effect

((Discovery))

In a preliminary investigation in 1921 of the free paths of electrons of very low energy (0.75 eV to 1.1 eV) in various gases, Ramsauer found the free paths of these electrons in Ar gas to be very much greater that that calculated from gas-kinetic theory. It was found that the effective cross-section (proportional to the reciprocal of the free path) of Ar gas increases with decreasing velocity until the electron energy becomes less than 10 eV. For electron energies below this value, it decreases again to the lowest value found in the preliminary measurements.

Independently, Townsend and Bailey examined the variation of the free path with velocity for electrons with energies between 0.2 and 0.8 eV by a different method, and showed that a maximum of the free path occurs at about 0.39 eV. This was confirmed by much later work of Ramsauer and Kollath. After these classical experiments, the behavior of a large number of gases and vapors has been examined over a wide voltage range. The striking features of the cross-section vs velocity curves are their variation in shape and size and also the marked similarity of behavior of similar atoms, such as those of the heavier rare gases and the alkali metal vapors. At the time of the earlier measurements no satisfactory explanation of the phenomena could be given, but on the introduction of quantum mechanics it was immediately suggested that the effect was a diffraction phenomenon.

The Ramsauer-Townsend effect can be observed as long as the scattering does not become inelastic by excitation of the first excited state of the atom. This condition is best fulfilled by the closed shell noble gas atoms. Physically, the Ramsauer-Townsend effect may be thought of as a diffraction of the electron around the rare-gas atom, in which the wave function inside the atom is distorted in just such a way that it fits on smoothly to an undistorted wave function outside. The effect is analogues to the perfect transmission found at particular energies in one-dimensional scattering from a square well.

Note that the Born approximation is not applicable to the low-energy collisions of electron with atoms, and the experimental results obtained in this limit clearly show that a more sophisticated theory (in this case, phase shift analysis) is required. We note that the Ramsauer-Townsend experiment as well as the Franck-Hertz experiment (mainly inelastic scattering) is now introduced in the Advance laboratory course of the universities

((**Experiment**))

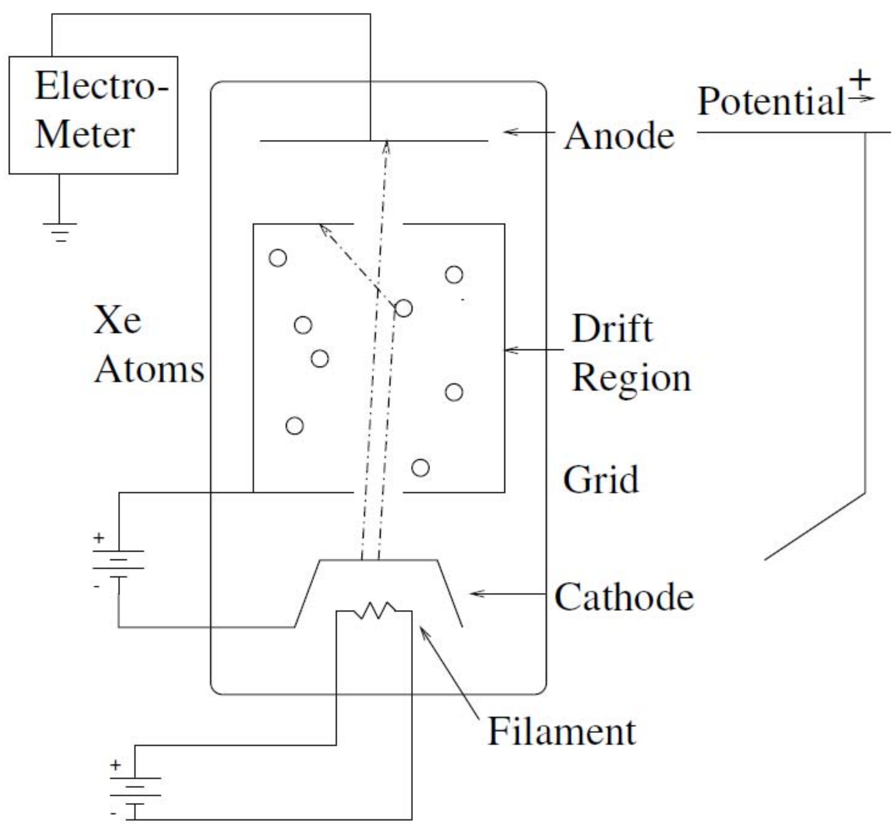


Fig. Schematic diagram for the apparatus for measuring scattering cross-section. Xenon in vapor. This apparatus (as one of the Advanced Laboratory in universities) is used to measure the elastic scattering cross-section for low energy electrons (0 - 5 eV) since for high energies inelastic scattering (excitation) dominates ($E_0 \approx 10$ eV).

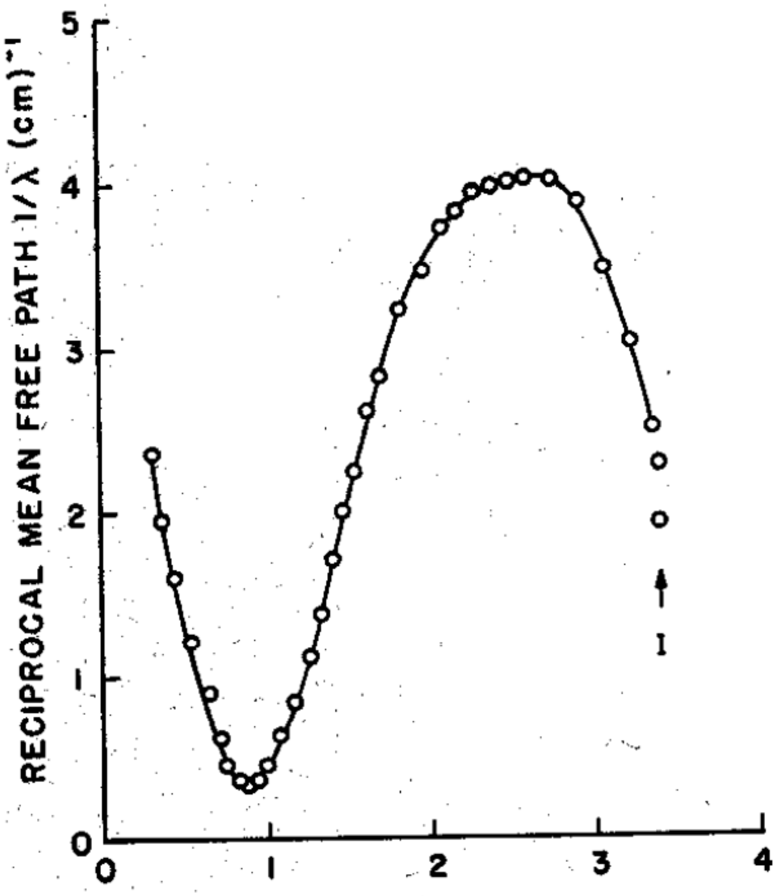


Fig. Typical results on the Ramusauer-Townsend experiment for Xenon gas. The cross section times density as a function of $\sqrt{V}$. V is the electron energy. Ionization occurs at the position denoted by *I*. (Kukolich).

((**Note**)) **Comparison between Frank-Hertz experiment and Ramsauer-Townsend experiment**

The Ramsauer-Townsend experiment is similar to the Frank-Hertz experiment. The difference between these two experiments is as follows. For the Frank-Hertz experiment, the collision between atoms and electrons is inelastic. The energy of the bombarding electron is lost because of the ionization process of atoms (such as Hg vapor). The electrons in atoms undergo transitions from the lower states to the more excited state. For the Ramsuer-Townsend experiment, on the other hand, the electrons are elastically scattered by atoms (such as Xenon gas). The origin of this effect is the diffraction of electron waves by atoms.

REFERENCES

N.F. Mott and H.S.W. Massey, The Theory of Atomic Collisions, 3rd edition (Oxford. 1965).

D. Bohm, Quantum Theory (Dover, 1989).
S.G. Kukolich, Am. J. Phys. 36 (8) 701, "Demonstration of the Ramsauer-Townsend Effect in a Xenon Thyratron."

13. Comment on Ramsauer Effect ((by D. Bohm))

We observe from eq. (1) that if the scattering phase is equal to some integral multiple of π for nonzero *k*, the cross section vanishes. If δ_0 is an integral multiple of *π*, then $\tan\delta_0 = 0$. For a square well, we obtain the condition for the vanishing of $\tan\delta_0$ from eq. (2):

$$\frac{\tan(\kappa_s R)}{\kappa_s R} = \frac{\tan(kR)}{kR}.$$

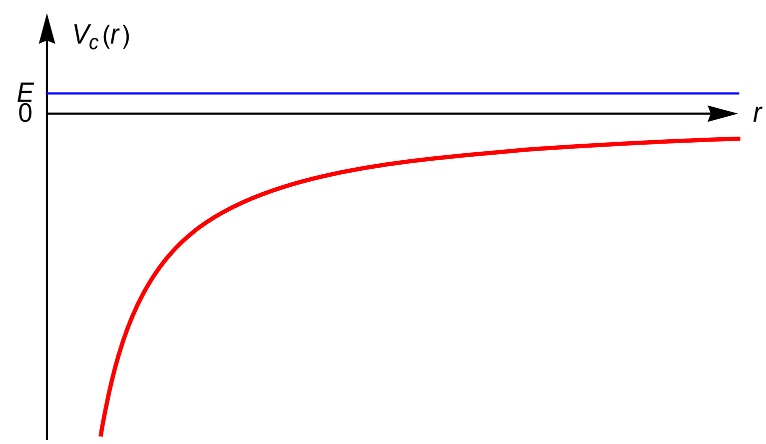
For small *k*, $kR << 1$. Replacement of $\tan kR$ by kR then yields

$$\tan(\kappa_s R) \approx \kappa_s R$$

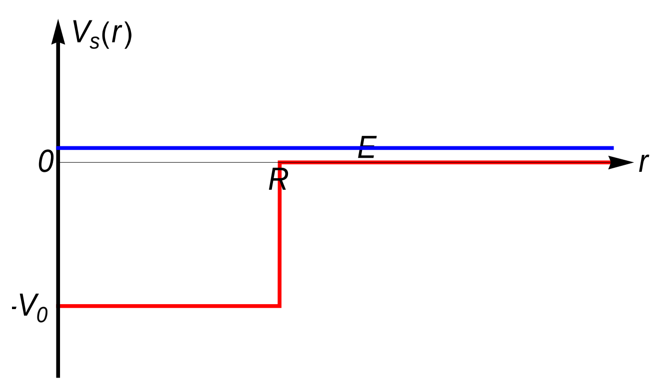
For small *k*, κ_s is given approximately by $\sqrt{2\mu V_0/\hbar^2}$. If V_0 and *R* are such that the eq. (4) is satisfied, the scattering cross section will be zero, and if it is nearly satisfied, the cross section will be very small. This vanishing of the scattering cross section for a non-zero potential is peculiar to the wave properties of matter. It would occur, for example, with light waves which were being scattered from small transparent spheres with a high index of refraction, so. chosen that the $\sin\delta_0$ corresponding to the scattered wave vanished. This means, essentially, that the contributions of the various parts of the potential to the scattered wave interfere destructively, leaving only an un-scattered wave. Although this result was derived for a square well, it can easily be extended to any well that has the property that it is fairly localized in space. This is because the vanishing of the phase is determined by the cumulative phase shifts suffered by the wave throughout the entire well, so that it is always possible to obtain a phase shift of $n\pi$ by properly choosing the magnitude and range of the potential. For slow electrons scattered from noble gas atoms, it turns out that $\sin\delta_0$ is very small and the cross section for electron-atom scattering is therefore much smaller than the gas-kinetic cross section. This effect is known as the Ramsauer effect. As the electron energy is increased, the phase of the scattered wave changes, and, eventually, at higher energies above 25 eV the usual gas-kinetic cross section is approached.

The Ramsauer effect is somewhat analogous to the transmission resonances obtained in the one dimensional potential. The analogy, however, is not complete, because the condition for the Ramsauer effect [eq. (4)] is not exactly the same as that for a transmission resonance in a one-dimensional well. The reason for the difference is that in the one-dimensional case we define the transmitted wave as the total wave that comes through the well. In the scattering problems, we have an incident wave that converges on the well. Some of it enters the well and some of it is reflected at the edge of the well. The net effect is to produce an outgoing wave, whose phase depends on what happens to the wave at the well. The question of how much of this outgoing wave corresponds to a scattered wave depends on how large a phase shift it has suffered relative to the outgoing wave which would have been present in the absence of a potential. Thus we see that the intensity of the scattered wave depends on properties of the potential that are somewhat different from those determining the intensity of that part of the wave that is transmitted through the potential and out again on the other side. The vanishing of the cross section in the Ramsauer effect is, as we have already seen, a result of the fact that the contributions of different parts of the potential all add up in such a way as to produce a wave that cannot be distinguished from one which has not been inside a potential at all.

14. Origin of the meta-stable bound states



Suppose that the energy of the particle (E) is a little higher than zero energy. In the case of attractive Coulomb potential, the potential $V_c(r)$ is negative and smoothly increases with decreasing the distance r. There is no drastic change of $V_c(r)$ at any r. Thus the particle with the energy E (>0) (even if E is very small) leak outside the effective range of the potential without ant reflection. Thus it does not become a bound state.



How about the attractive square-well potential, there is a drastic change in the form of the potential $V_{sq}(r)$ at the wall of $r = R$. Thus a part of particles with the energy E undergoes reflections at $r = R$. The remaining particles leak and transmit outside the potential. The cause of such reflections is due to the drastic change of the wavenumber in the wave function at $r = R$. Particles having reflections at the wall of the potential attempt to transmit the outside of the potential wall, and finally succeed in leaking the potential. As a result of such a repetition of reflections, particles are temporally bound inside the well of the potential, forming the meta-stable state as a positive eigenvalue. Note that this state is not the same as the bound state of negative energy

15. The phase shift δ_0 for the S-wave scattering

We consider the phase shift for the S-wave scattering.
From

$$\tan(kR+\delta_0) = \frac{\tan(kR)+\tan\delta_0}{1-\tan(kR)\tan\delta_0} = \frac{kR}{\kappa R}\tan(\kappa R),$$

we get the phase shift as

$$\tan\delta_0 = \frac{\dfrac{kR}{\kappa_s R}\tan(\kappa_s R) - \tan(kR)}{1+\dfrac{kR}{\kappa_s R}\tan(\kappa_s R)\tan(kR)}$$

and the total scattering cross section is given by

$$\sigma_0 = \frac{4\pi}{k^2}\sin^2\delta_0 .$$

Here we define

$$\frac{kR}{\kappa_s R}\tan(\kappa_s R) = \tan(qR)$$

where q is a wavenumber which is newly introduced. Then we get

$$\tan\delta_0 = \frac{\tan(qR)-\tan(kR)}{1+\tan(qR)\tan(kR)} = \tan(qR-kR)$$

or

$$\delta_0 = qR - kR = \arctan[\frac{kR}{\kappa_s R}\tan(\kappa_s R)] - kR \approx kR[\frac{\tan(\kappa_s R)}{\kappa_s R} - 1] \qquad (\text{mod } \pi)$$

with the condition

$$(\kappa_s R)^2 = (kR)^2 + (k_0 R)^2$$

and

$$U_0 = \frac{2\mu}{\hbar^2}V_0 = k_0^{\,2}$$

At very low energies, using $\tan x \approx x$ for $x << 1$, we get

$$\delta_0 = qR - kR = kR(\frac{\tan(\kappa_s R)}{\kappa_s R} - 1)$$

We imagine that we are slowly deepening the potential well (V_0 is increasing slowly)

(i) $\kappa_s R = 0$

$\delta_0 = 0$, which means $\sigma_0 = 0$.

(ii) $\kappa_s R = \pi/2$

(the attractive square well just meets the criterion to host a single S-wave bound state)

$\tan(\kappa_s R) \to \infty$,

and

$$\tan\delta_0 = \frac{\frac{kR}{\kappa R}\tan(\kappa_s R) - \tan(kR)}{1 + \frac{kR}{\kappa R}\tan(\kappa_s R)\tan(kR)} \approx \frac{1}{\tan(kR)} \approx \frac{1}{kR} \to \infty .$$

Then δ_0 goes through $\pi/2$. In this case a bound state at zero energy is like a resonance. σ_0 takes a maximum value (we will discuss later); $\sigma_0 = \frac{4\pi}{k^2}$, which is dependent on k.

(iii) $\kappa_s R = \pi$,

$\tan\delta_0 = -\tan(kR) = -kR$,

δ_0 is nearly equal to π. σ_0 becomes zero.

(iv) $\kappa_s R = 3\pi/2$
(the potential becomes capable of hosting a second bound state, and there is another resonance).

$\tan(\kappa_s R) \to -\infty$,

and

$$\tan\delta_0 = \frac{\frac{kR}{\kappa_s R}\tan(\kappa_s R) - \tan(kR)}{1 + \frac{kR}{\kappa_s R}\tan(\kappa_s R)\tan(kR)} \approx \frac{1}{\tan(kR)} = \frac{1}{kR} \to +\infty .$$

Then δ_0 goes through $3\pi/2$. σ_0 takes a maximum value.

(v) $\kappa_s R = 2\pi$

$\tan(\kappa_s R) \to 0$,

or

$\tan\delta_0 = -\tan(kR) = -kR$,

So δ_0 is nearly equal to 2π. σ_0 becomes zero.

Note that when $\kappa_s R = n\pi$, the scattering cross section vanishes identically and the target becomes invisible ($\sigma_0 = 0$, the ***Ramsauer-Townsend effect***).

We draw the plot of $y = \delta_0$ vs $x = \kappa_s R$ with kR (= a =0.05, $E_s = \frac{\hbar^2}{2\mu}k^2 \approx 0$) as a parameter by using Mathematica. For convenience the value of kR is fixed as a small value.

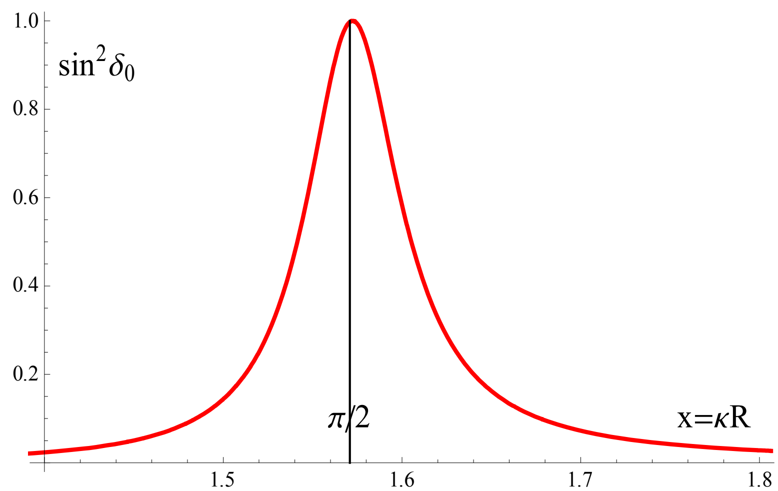
$y_0 = \delta_0 = \arctan[\frac{a}{x}\tan(x)] - a$

$a = kR$, $\quad x = \kappa_s R = \sqrt{k^2 R^2 + k_0{}^2 R^2} = \sqrt{a^2 + k_0{}^2 R^2}$,

In the low energy limit, $x \approx a_0 = k_0 R$

$$y = \delta_0 = \begin{cases} y_0 & (0 < x < \pi/2) \\ y_0 + \pi & (\pi/2 < x < 3\pi/2) \\ y_0 + 2\pi & (3\pi/2 < x < 5\pi/2) \\ y_0 + 3\pi & (5\pi/2 < x < 7\pi/2) \\ y_0 + 4\pi & (7\pi/2 < x < 9\pi/2) \end{cases}$$

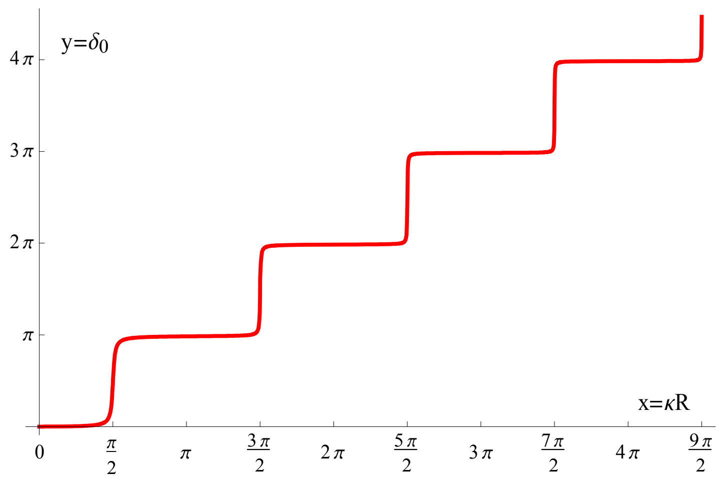
We also calculate the value of $\sin^2 \delta_0$ as a function of *x*. The total cross section shows a sharp peak at $x = \kappa_s R = \pi/2$.



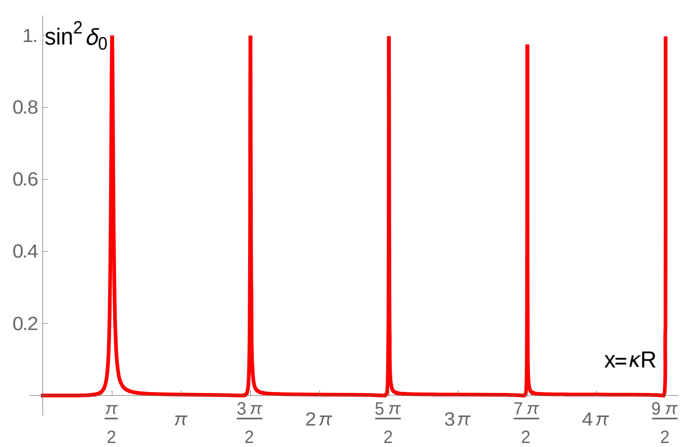
((**Mathematica**))

```
Clear["Global`*"]; a = 0.05; k1 = ArcTan[a/x Tan[x]] - a;
y = Which[0 < x < π / 2, k1, π / 2 < x < 3 π / 2, k1 + π,
   3 π / 2 < x < 5 π / 2, k1 + 2 π, 5 π / 2 < x < 7 π / 2, k1 + 3 π,
   7 π / 2 < x < 9 π / 2, k1 + 4 π];

f1 = Plot[Evaluate[y], {x, 0, 7 π},
   Ticks → {Range[0, 5 π, π / 2] , Range[0, 5 π, π]} ,
   PlotStyle → {Red, Thick}, PlotPoints → 60] ;
f2 = Graphics[{Text[Style["x=κR", Black, 12], {8.5 π / 2, 0.8}],
    Text[Style["y=δ0", Black, 12], {1, 4.2 π}]}];
Show[f1, f2, PlotRange → All]
```




```
h1 = Plot[Evaluate[Sin[y]^2, {x, 0, 7 π} ], PlotStyle → {Red, Thick},
  PlotPoints → 100,
  Ticks → {Range[0, 5 π, π / 2], Range[0, 1, 0.2] } ,
  PlotRange → All] ;
h2 = Graphics[{Text[Style["x=κR", Black, 12], {8.5 π / 2, 0.1}],
   Text[Style["sin^2δ0", Black, 12], {0.8, 1}]}];
Show[h1, h2, PlotRange → All]
```



((**Summary**))

The above results are summarized in two figures. In order to draw these figures, we use the Gaussian distribution function and the Heaviside step function, which are defined by

$$f_1(x) = \frac{1}{\sqrt{2\pi}\sigma}\exp(-\frac{x^2}{2\sigma^2}) \text{ and } f_2(x) = \frac{1}{2}[1 + erf(\frac{x}{\sqrt{2}\sigma})],$$

with $\sigma = 0.1$.

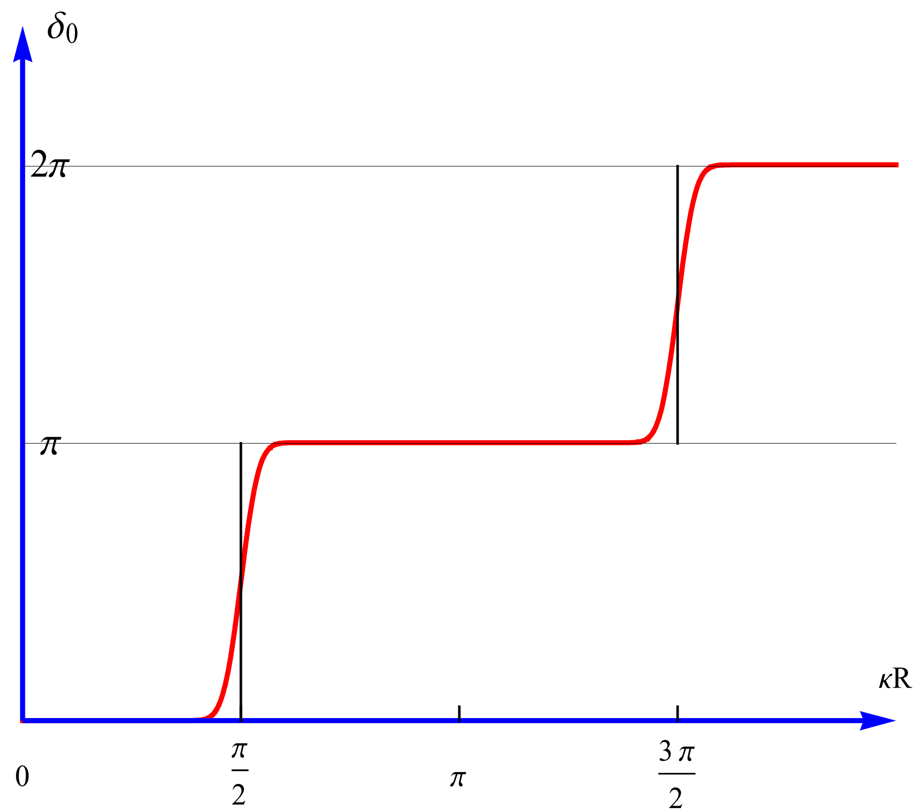


Fig. Schematic diagram. The phase shift δ_0 vs $\kappa_s R$. δ_0 shows a drastic change in the vicinity of $\kappa_s R = \frac{\pi}{2}(2n+1)$, which means that $\kappa_s R \approx k_0 R = a_0 = \frac{\pi}{2}(2n+1)$ in the low energy limit.

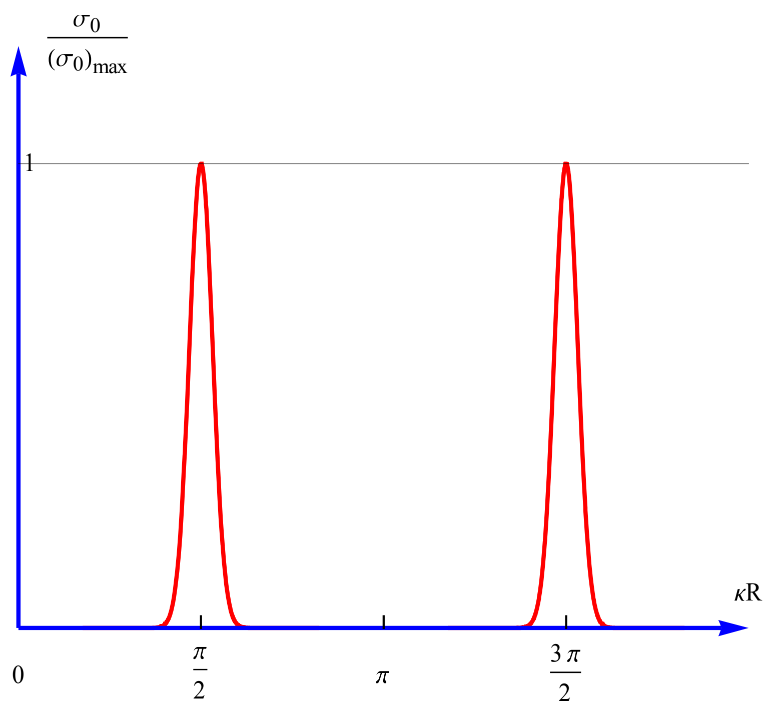
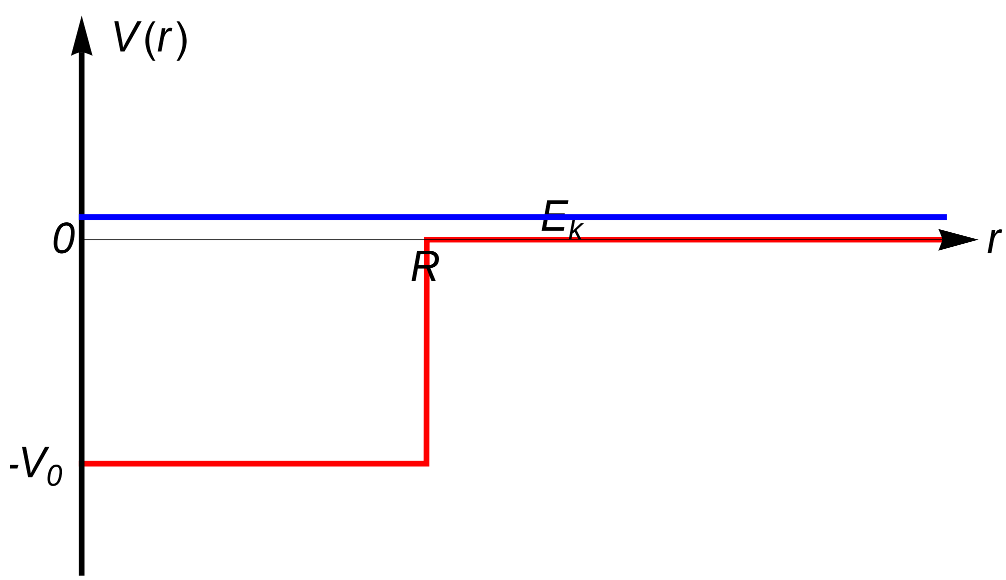


Fig. $\sin^2\delta_0$ vs $\kappa_s R$. It shows a sharp peak in the vicinity of $\kappa_s R = \frac{\pi}{2}(2n+1)$.

16. Attractive square-well potential-III: graphical solution (ContourPlot)



We consider the solution of two equations given by

$$(\kappa_s R)^2 = (kR)^2 + U_0 R^2$$

$$\tan(kR+\delta_0)=\frac{k}{\kappa_s}\tan(\kappa_s R)=\frac{kR}{\kappa_s R}\tan(\kappa_s R)$$

For simplicity, we have

$$U_0R^2=(k_0R)^2={a_0}^2 \qquad \text{or} \qquad a_0=k_0R$$

$$U_0=\frac{2\mu}{\hbar^2}V_0={k_0}^2, \qquad E_s=\frac{\hbar^2}{2\mu}k^2$$

Note that a_0 is the depth of attractive potential. The number of bound states strongly depends on the magnitude of a_0 (this will be discussed in association with the Levinson's theorem). We also define as

$$y=kR, \qquad x=\kappa_s R.$$

Then we get two equations such that

$$x^2=y^2+{a_0}^2 \tag{1}$$

$$x\tan(y+\delta_0)=y\tan(x). \tag{2}$$

We note that

$$\tan(y+\pi)=\tan y$$

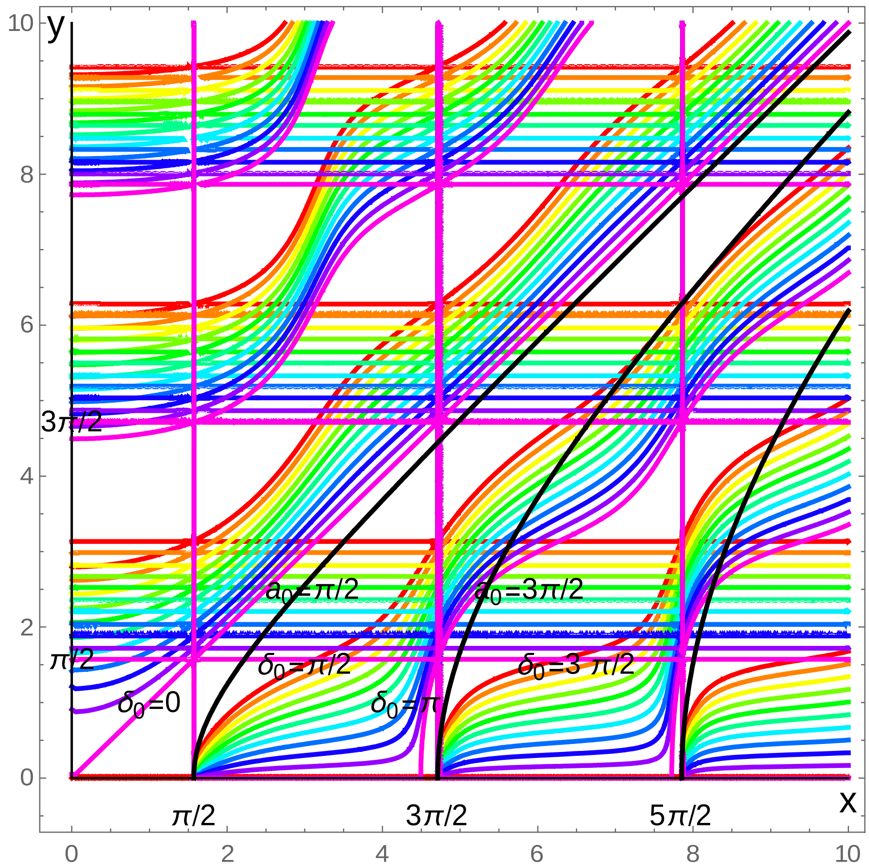
For $\delta_0=\theta_0+n\pi$ ($0<\theta_0<\pi$)

$$\tan(y+\delta_0)=\tan(y+\theta_0+n\pi)=\tan(y+\theta_0)$$

Thus the ContourPlot of $x\tan(y+\theta_0)=y\tan(x)$ is the same as that of

$$x\tan(y+\theta_0+n\pi)=y\tan(x).$$

We solve this problem using the Mathematica graphically. We make a plot of Eqs.(1) and (2) using the ContourPlot for x vs y for various δ_0, where a_0 is a fixed parameter.


y
x
10
8
6
4
2
0
0
2
4
6
8
10
3π/2
π/2
π/2
3π/2
5π/2
δ0=0
δ0=π/2
δ0=π
δ0=3 π/2
a0=π/2
a0=3π/2

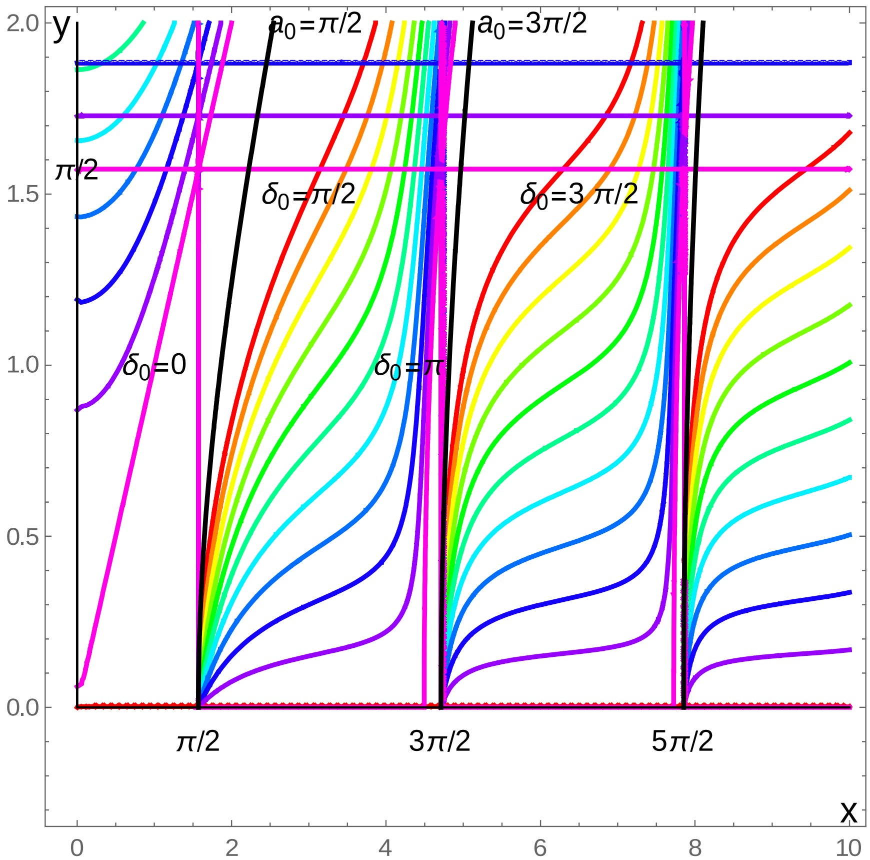
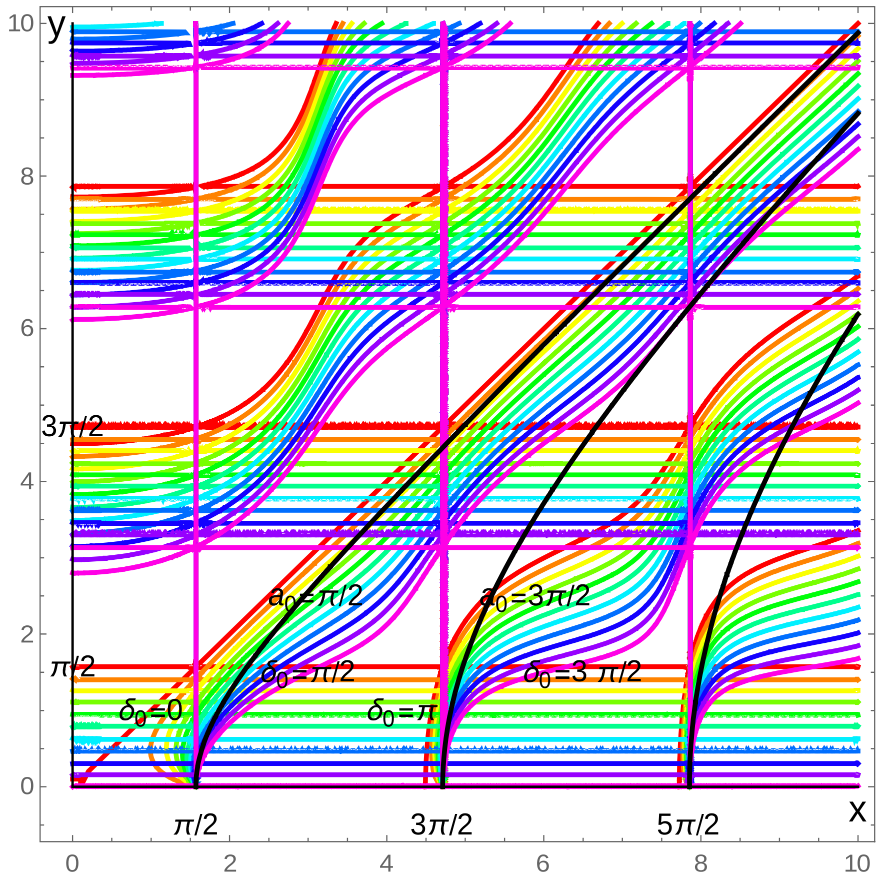


Fig. ContourPlot of x vs y. $y = kR$ and $x = \kappa_s R$. a_0 = $\pi/2$, $3\pi/2$. and $5\pi/2$ (black lines). δ_0 = π/2 (red), 0.55π, 0.6π, 0.65 π, 0.7 π, 0.75π, 0.8π, 0.85 π, 0.9 π, 0.95π, and π. δ_0 = 3π/2 (red), 1.55π, 0.6π, 1.65 π, 1.7 π, 1.75π, 1.8π, 1.85 π, 1.9 π, 1.95π, and 2π. The horizontal lines between y = $\pi/2$ and π (independent of x) are the trivial solutions derived from the present ContourPlot calculation.


y
x
3π/2
π/2
a_0=π/2
a_0=3π/2
δ_0=0
δ_0=π/2
δ_0=π
δ_0=3 π/2
π/2
3π/2
5π/2

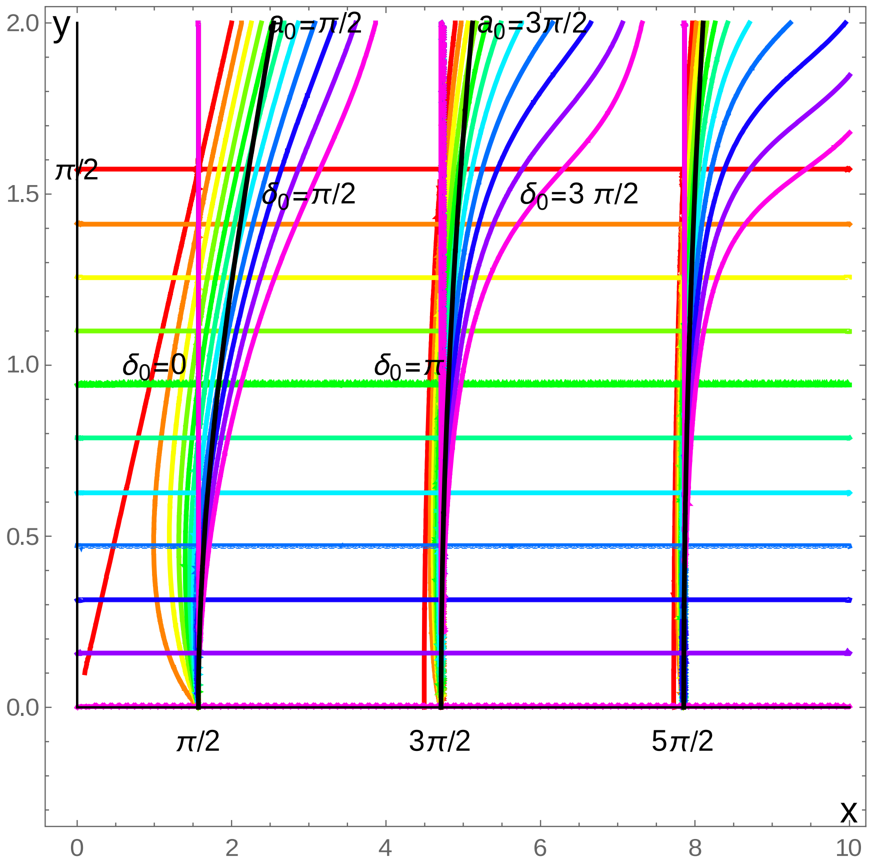


Fig. ContourPlot of x vs y. $y = kR$ and $x = \kappa_s R$. $a_0 = \pi/2$, $3\pi/2$. and $5\pi/2$ (black lines). $\delta_0 = 0$ (red), 0.05π, 0.1π, 0.15 π, 0.2 π, 0.25π, 0.3π, 0.35 π, 0.4 π, 0.45π, and π/2. $\delta_0 = \pi$ (red), 1.05π, 1.1π, 1.15 π, 1.2 π, 1.25π, 1.3π, 1.35 π, 1.4 π, 1.45π, and 3π/2. The horizontal lines between y = 0 and π/2 (independent of x) are the trivial solutions derived from the present ContourPlot calculation.

((**Discussion**))

There is a significant exception to this independent of the cross section on energy. Suppose that

$$\kappa_s R = \sqrt{k^2 R^2 + k_0{}^2 R^2} \approx k_0 R = \frac{\pi}{2}$$

In the above figure, this corresponds to the case of [$x = \frac{\pi}{2}$, $y = 0$, $a_0 = k_0 R = \frac{\pi}{2}$, $\delta_0 = \frac{\pi}{2}$],

Then we have

$$\tan(kR + \delta_0) = \frac{kR}{\kappa_s R}\tan(\kappa_s R) \rightarrow \infty$$

or

$$kR + \delta_0 = \frac{\pi}{2}$$

or

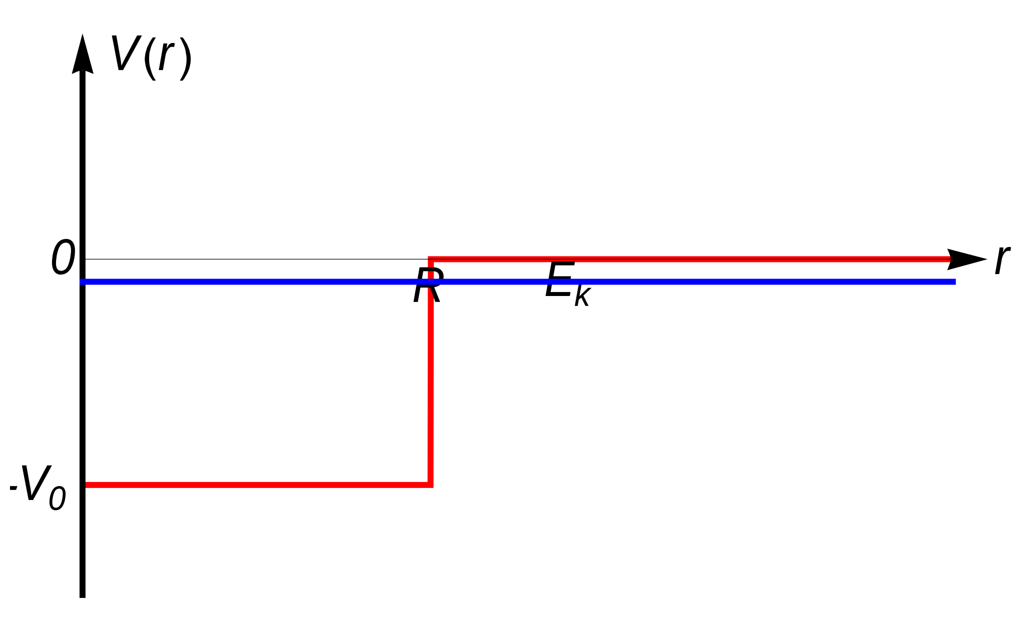
$$\delta_0 \approx \frac{\pi}{2},$$

since $kR << 1$. The total cross section takes a maximum as

$$\sigma_{tot} = \sigma_{l=0} = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2} = 4\pi R^2 \frac{1}{k^2 R^2},$$

leading to the occurrence of the zero-energy resonance. We see a pronounced dependence of the total cross section on energy. The magnitude of the total cross section is much larger than that given before when $k \to 0$, $E \to 0$.

17. Attractive square-well potential-I: bound states and S-wave resonance



We consider the case when $E_b = -\frac{\hbar^2}{2\mu}\alpha^2 = -\varepsilon$ (<0) for the attractive square-well potential. α is close to zero and real.

((**Bound state of a deuteron**))

E coincides with the energy eigenvalue of the bound state. Note that the bound state of a deuteron is E = -2.23 MeV. The value of α for a bound state is easily calculated from the fact that outside the potential the wave function is just a decaying exponential (for *S* waves),

$$\psi = A\frac{1}{r}\exp(-\alpha r),$$

where

$$\alpha = \sqrt{\frac{2\mu B}{\hbar}}$$

and *B* is the binding energy of the deuteron. Thus we obtained for the value of α in the bound state.

The wave function inside the well has gone past a maximum and is decreasing with radius to meet a decaying exponential at $r = R$. Now, the potential is of the order of 20 MeV deep; hence α undergoes only a small change as *E* is increased from -2.23 MeV to a value of zero or slightly above, simply because the wavelength at any particular point is not changed much by this small fractional increase in kinetic energy. [**Bohm D., Quantum Theory**].

Here we consider the case for $l = 0$ (S wave)

(i) Schrödinger equation for $r<R$

$$-\frac{\hbar^2}{2\mu}\frac{d^2u}{dr^2} - V_0 u = Eu = (-\varepsilon)u = -\frac{\hbar^2\alpha^2}{2\mu}u$$

or

$$\frac{d^2u}{dr^2} + \frac{2mV_0}{\hbar^2}u = \alpha^2 u$$

or

$$u'' + (-\alpha^2 + k_0{}^2)u = 0$$

or

$$u'' + \kappa_b{}^2 u = 0$$

where

$$\frac{2\mu V_0}{\hbar^2} = U_0 = k_0{}^2,$$

$$\kappa_b{}^2 = -\alpha^2 + k_0{}^2.$$

Then we get the solution as

$$u = B\sin(\kappa_b r),$$

with the boundary condition, $u(r) = 0$.

(ii) Schrödinger equation for *r*>*R*

$$u'' - \alpha^2 u = 0,$$

or

$$u = Ae^{-\alpha r}.$$

The boundary condition at $r = R$, leads to

$$B\sin(\kappa_b R) = Ae^{-\alpha R},$$

$$B\kappa\cos(\kappa_b R) = -A\alpha e^{-\alpha R}.$$

Then we have

$$\kappa_b R\cot(\kappa_b R) = -\alpha R,$$

with

$$\kappa_b{}^2 + \alpha^2 = k_0{}^2.$$

We determine the constants *A* and *B*.

$$A = \frac{2e^{\alpha R}\sqrt{\kappa_b R\alpha R}\sin(\kappa_b R)}{\sqrt{R}\sqrt{2\kappa_b R\alpha R + 2\kappa_b R\sin^2(\kappa_b R) - 2\alpha R\sin(2\kappa_b R)}}$$

$$B = \frac{2\sqrt{\kappa_b R\alpha R}}{\sqrt{R}\sqrt{2\kappa_b R\alpha R + 2\kappa_b R\sin^2(\kappa_b R) - 2\alpha R\sin(2\kappa_b R)}}$$

from the normalization of the wave function. Note that the constants A and B are in the units of $cm^{-1/2}$.

We solve the problem using the Mathematica.

$$x = \kappa_b R, \qquad y = \alpha R$$

In this case,

$$y = -x \cot x, \qquad x^2 + y^2 = k_0^2 R^2 = a_0^2$$

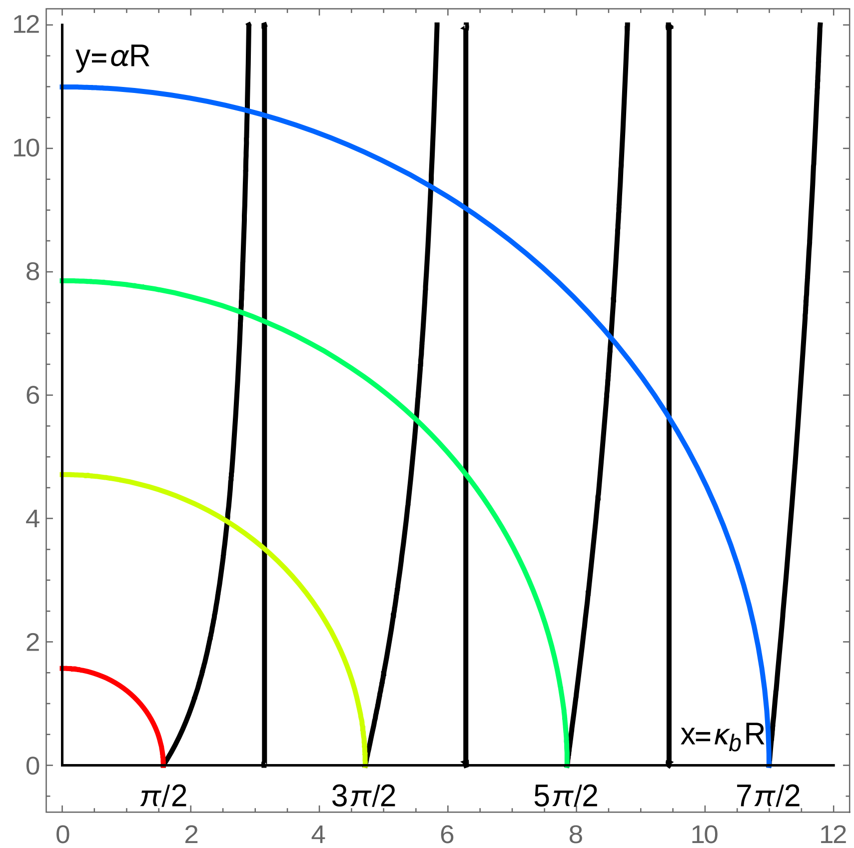


Fig. Plot of $y = -x \cot x$ (red line) and $x^2 + y^2 = a_0^2 = (k_0 R)^2$. $a_0 = \pi/2$, $a_0 = 3\pi/2$ (light green line), $a_0 = 5\pi/2$ (green line), and $a_0 = 7\pi/2$ (blue line), $x = \kappa_b R$. $y = \alpha R$. One bound state for $a_0 = \pi/2$. Two bound states for $a_0 = 3\pi/2$. Three bound states for $a_0 = 5\pi/2$) As a_0 increases, the potential well becomes deep.

The solution is the intersection of $y = -x \cot x$ (red line) and $x^2 + y^2 = a_0^2$ ($a_0 = \pi/2$; blue line).

$$x = \frac{\pi}{2}, \qquad y = 0, \qquad a_0 = \frac{\pi}{2}.$$

implying that

$$a_0 = k_0 R = \frac{\pi}{2},$$

$$U_0 = k_0{}^2 = \left(\frac{\pi}{2R}\right)^2,$$

The energy eigenvalue E is

$$E_b = -\varepsilon = -\frac{\hbar^2}{2m}\alpha^2 \to 0 \qquad \text{(quasi-bound state)}$$

When the radius a_0 is slightly larger than $\pi/2$, the intersection of two curves is seen at $y>0$. Since $y = \alpha R$, α comes to take a small positive value. In this case $(-\varepsilon)$ slightly becomes negative, forming the bound state. For $0 < a_0 < \frac{\pi}{2}$, there is no bound state.

(i) $a_0 = \frac{\pi}{2}$. One bound state with $E_b = 0$.

$$x = \kappa_b R = \frac{\pi}{2}, \; y = \alpha R = 0$$

(ii) $\frac{\pi}{2} < a_0 < \frac{3\pi}{2}$. One bound state with $E_b = -\varepsilon = -\frac{\hbar^2}{2m}\alpha^2 < 0$

(iii) $a_0 = \frac{3\pi}{2}$. One bound state with $E_b = 0$. One bound state with $E_b = -\varepsilon = -\frac{\hbar^2}{2m}\alpha^2 < 0$

$x = 2.56582$, $y = 3.95262$
$x = \pi/2$, $y = 0$

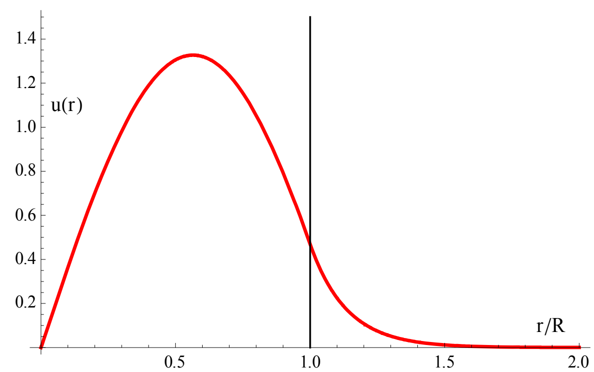


Fig. Plot of $u(r)$ vs r/R for the bound states with $x = \kappa_b R = 2.56582$, $y = \alpha R = 3.95262$. $a_0 = \frac{3\pi}{2}$.

(iv) $\frac{3\pi}{2} < a_0 < \frac{5\pi}{2}$. Two bound state with $E_b = -\varepsilon = -\frac{\hbar^2}{2m}\alpha^2 < 0$.

(v) $a_0 = \frac{5\pi}{2}$. One bound state with $\alpha = 0$. Two bound state with $E_b = -\varepsilon = -\frac{\hbar^2}{2m}\alpha^2 < 0$

$x = 2.77982$, $y = 7.34559$
$x = 5.50627$, $y = 5.60053$
$x = 5\pi/2$, $y = 0$

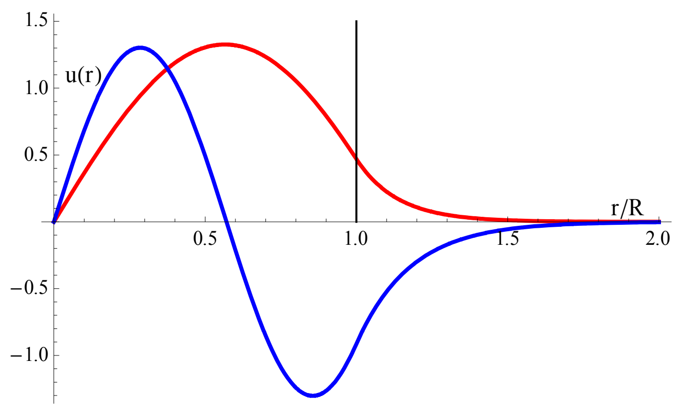


Fig. Plot of $u(r)$ vs r/R for the bound states with $x = 2.77982$, $y = 7.34559$ (red), and $x = \kappa_b R = 5.50627$, $y = \alpha R = 5.60053$ (blue). $a_0 = \frac{5\pi}{2}$

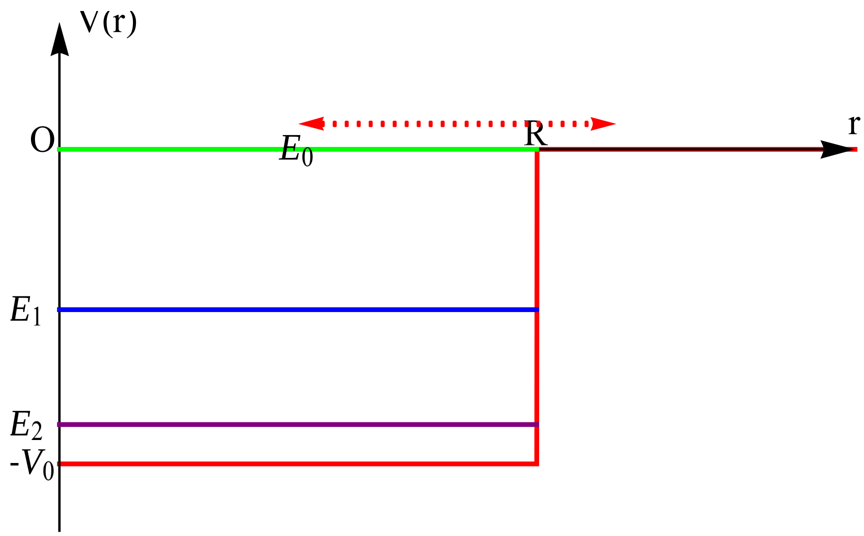


Fig. $a_0 = \frac{5\pi}{2}$. Bound states with E_1 and E_2. Quasi bound state with $E_b \approx 0$. The particle with $E_b \approx 0$ will go outside from the inside of the square-well potential through a tunneling effect.

(vi) $a_0 = \frac{7\pi}{2}$. One bound state with $\alpha = 0$. Three bound state with $E_b = -\varepsilon = -\frac{\hbar^2}{2m}\alpha^2 < 0$

$x = 2.87687$, $y = 10.6126$
$x = 5.73454$, $y = 9.38187$
$x = 8.53599$, $y = 6.93196$
$x = 7\pi/2$, $y = 0$

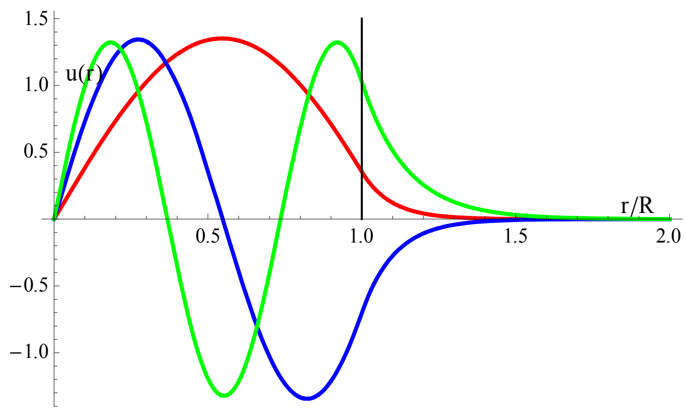


Fig. Plot of $u(r)$ vs r/R for the bound states with. $x = \kappa_b R = 2.87687$, $y = \alpha R = 10.6126$ (red), $x = 5.73454$, $y = 9.38187$ (blue), and $x = 8.53599$, $y = 6.93196$ (green). $a_0 = \frac{5\pi}{2}$

16. Connection between scattering amplitude and binding energy

We start with the total cross section for the S wave scattering,

$$\sigma_{tot} = 4\pi R^2 [\frac{\tan(\kappa_s R)}{\kappa_s R} - 1]^2,$$

where

$$E_s = \frac{\hbar^2}{2\mu}k^2, \quad k_0^{\ 2} = \frac{2\mu V_0}{\hbar^2}.$$

Suppose that a positive energy E_s of the particle (scattering) shifts to a negative energy E_b (bound state)

$$E_s = \frac{\hbar^2}{2\mu}k^2 \quad \to E_b = -\frac{\hbar^2}{2\mu}\alpha^2,$$

where *s* denotes the scattering problem and *b* denotes the bound state problem. Effectively this means that the replacement of the wavenumber occurs as $k \to i\alpha$ in this process. Correspondingly the wavenumber changes as

$$\kappa_s = \sqrt{k_0^2 + k^2}, \qquad \to \kappa_b = \sqrt{k_0^2 - \alpha^2}.$$

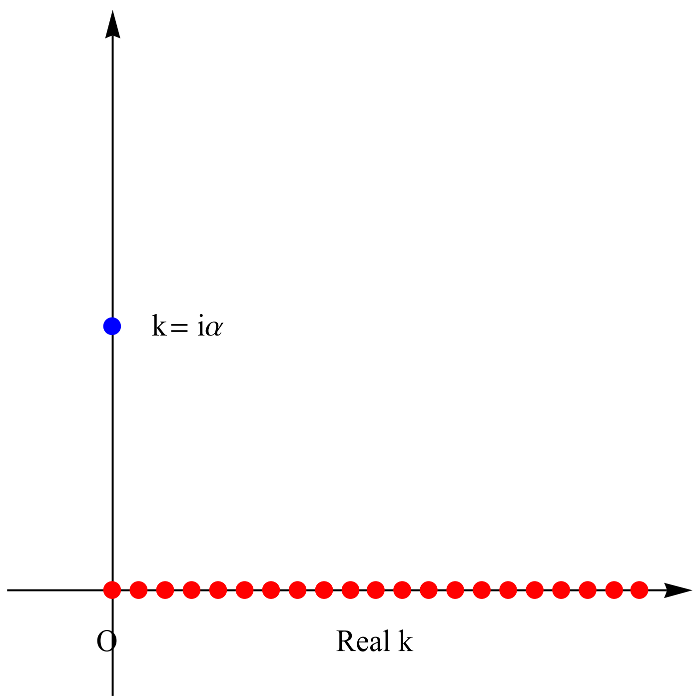


Fig. The complex *k*-plane with bound-state pole at $k = i\alpha$. Region of physical scattering is denoted by real *k* (>0) (scattering state).

After this replacement, the scattering problem is reduce to the bound-state problem which is discussed above. The boundary condition of the bound-state problem is given by

$$\kappa_b R\cot(\kappa_b R) = -\alpha R.$$

Then we have

$$\left(\frac{\tan(\kappa_s R)}{\kappa_s R}\right)_{scatt} \approx \left(\frac{\tan(\kappa_b R)}{\kappa_b R}\right)_{bound} = -\frac{1}{\alpha R}.$$

For $\alpha R << 1$, we get

$$\sigma_{tot} \approx 4\pi R^2 \left(\frac{\tan(\kappa_s R)}{\kappa_s R} - 1 \right)^2$$
$$= 4\pi R^2 (-1 - \frac{1}{\alpha R})^2$$
$$= \frac{4\pi}{\alpha^2}(1+\alpha R)^2$$
$$\approx \frac{4\pi}{\alpha^2}(1+2\alpha R)$$

Such a method (the analytical continuity) allows one to bypass the problem of determining the potential and then calculating the cross section. This method only works when α is very small.

((**Summary**))

Scattering state	Bound state
k	$i\alpha$
$E_s = \frac{\hbar^2 k^2}{2\mu}$	$E_b = -\frac{\hbar^2 \alpha^2}{2\mu}$
$\kappa_s = \sqrt{k^2 + k_0^2}$	$\kappa_b = \sqrt{-\alpha^2 + k_0^2}$
$\kappa_s R = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots$ (resonance)	$\kappa_b R = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots$ (bound state)
$\kappa_s R \cot(\kappa_s R) = kR\cot(kR + \delta_0)$	$\kappa_b R \cot(\kappa_b R) = -\alpha R$
$\sigma_{tot} \approx 4\pi R^2 \left(\frac{\tan(\kappa_s R)}{\kappa_s R} - 1 \right)^2$	

As is shown below, we have

$$kR\cot(kR + \delta_0) \approx kR\cot\delta_0 = -\alpha - \frac{1}{2}k^2\alpha ,$$ (**Effective potential range**).

$$\sigma_{tot} = \frac{4\pi}{k^2}\sin^2\delta_0 = \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0} = \frac{4\pi}{k^2+\alpha^2}$$

18. Effective potential range-I (by H. Bethe) for attractive square-well potential

(a) Solution of the wave function u_s for $E_s = \frac{\hbar^2}{2m}k^2 > 0$

The wave function of scattering wave (s denotes scattering),

$$\frac{\partial^2 u_s}{\partial r^2} + (k^2 + k_0{}^2)u_s = 0$$ for 0<*r*<*R*

$$u_s(r) = A_s \sin(\kappa_s r),$$

$$\frac{\partial^2 u_s}{\partial r^2} + k^2 u_s = 0$$ for *r*>*R*

$$u_s(r) = B_s \sin(kr + \delta_0)$$

where

$$\kappa_s{}^2 = k^2 + k_0{}^2.$$

(b) Solution of the wave function u_b for $E_b = -\frac{\hbar^2}{2m}\alpha^2 < 0$

The wave function of scattering wave (*b* denotes the bound state)

$$\frac{\partial^2 u_b}{\partial r^2} + (-\alpha^2 + k_0{}^2)u_b = 0$$ for 0<*r*<*R*

$$u_b(r) = A_b \sin(\kappa_b r),$$

and

$$\frac{\partial^2 u_b}{\partial r^2} - \alpha^2 u_b = 0$$ for *r*>*R*

$$u_b(r) = B_b e^{-\alpha r},$$

where

$$\kappa_b{}^2 = -\alpha^2 + k_0{}^2$$

(c) Analytical continuation

Multiplying the first by u_s, the second by u_b, and subtracting, gives

$$[u_s \frac{\partial^2 u_b}{\partial r^2} + (-\alpha^2 + k_0{}^2)u_s u_b] - [u_b \frac{\partial^2 u_s}{\partial r^2} + (k^2 + k_0{}^2)u_b u_s] = 0,$$

or

$$(u_s \frac{\partial^2 u_b}{\partial r^2} - u_b \frac{\partial^2 u_s}{\partial r^2}) - (\alpha^2 + k^2) u_s u_b = 0 .$$

Integrating from 0 to R, we get

$$\int_0^R (u_s \frac{\partial^2 u_b}{\partial r^2} - u_b \frac{\partial^2 u_s}{\partial r^2}) dr - (\alpha^2 + k^2) \int_0^R u_s u_b dr = 0 ,$$

or

$$(u_s \frac{\partial u_b}{\partial r} - u_b \frac{\partial u_s}{\partial r})]_0^R = (\alpha^2 + k^2) \int_0^R u_s u_b dr .$$

Since $u_s(0) = u_b(0) = 0$, we have

$$(u_s \frac{\partial u_b}{\partial r} - u_b \frac{\partial u_s}{\partial r})_{r=R} = (\alpha^2 + k^2) \int_0^R u_s u_b dr .$$

Dividing by $u_s(R) u_b(R)$, we get

$$(\frac{1}{u_b} \frac{\partial u_b}{\partial r} - \frac{1}{u_s} \frac{\partial u_s}{\partial r})_{r=R} = \frac{(\alpha^2 + k^2)}{u_s(R) u_b(R)} \int_0^R u_s u_b dr .$$

The boundary condition of u_b at $r = R$;

$$\frac{1}{u_b} \frac{\partial u_b}{\partial r} |_{r=R-0} = \kappa_b \cot(\kappa_b R) , \qquad \frac{1}{u_b} \frac{\partial u_b}{\partial r} |_{r=R+0} = -\alpha ,$$

and

$$\frac{1}{u_b} \frac{\partial u_b}{\partial r} |_{r=R-0} = \frac{1}{u_b} \frac{\partial u_b}{\partial r} |_{r=R+0} ,$$

leading to the relation

$$\kappa_b \cot(\kappa_b R) = -\alpha . \qquad (1)$$

The boundary condition of u_s at $r = R$;

$$\frac{1}{u_s} \frac{\partial u_s}{\partial r} |_{r=R-0} = \kappa_s \cot(\kappa_s R) , \qquad \frac{1}{u_s} \frac{\partial u_s}{\partial r} |_{r=R+0} = k \cot(kR + \delta_0) ,$$

and

$$\frac{1}{u_s}\frac{\partial u_s}{\partial r}|_{r=R-0} = \frac{1}{u_s}\frac{\partial u_s}{\partial r}|_{r=R+0},$$

leading to

$$\kappa_s \cot(\kappa_s R) = k\cot(kR+\delta_0). \quad (2)$$

We note that

$$\left(\frac{1}{u_b}\frac{\partial u_b}{\partial r} - \frac{1}{u_s}\frac{\partial u_s}{\partial r}\right)_{r=R} = -\alpha - k\cot(kR+\delta_0) = \kappa_b \cot(\kappa_b R) - \kappa_s \cot(\kappa_s R)$$

Then we get the integral as

$$\begin{aligned} \frac{1}{u_s(R)u_b(R)}\int_0^R u_s u_b dr &= \frac{\kappa_b \cot(\kappa_b R) - \kappa_s \cot(\kappa_s R)}{\kappa_s^2 - \kappa_b^2} \\ &= \frac{\kappa_b \cot(\kappa_b R) - \kappa_s \cot(\kappa_s R)}{\alpha^2 + k^2} \end{aligned}.$$

or

$$\frac{(\alpha^2 + k^2)}{u_s(R)u_b(R)}\int_0^R u_s u_b dr = \kappa_b \cot(\kappa_b R) - \kappa_s \cot(\kappa_s R)$$

From Eqs.(1) and (2), we get

$$\kappa_s \cot(\kappa_s R) - \kappa_b \cot(\kappa_b R) = k\cot(kR+\delta_0) + \alpha.$$

We expand $\kappa_s \cot(\kappa_s R)$ around $\kappa_s = \kappa_b$ by using the Taylor expansion.

$$\begin{aligned} \kappa_s \cot(\kappa_s R) &= \kappa_b \cot(\kappa_b R) + [\cot(\kappa_b R) - \kappa_b R\csc^2(\kappa_b R)](\kappa_b - \kappa_b) + ... \\ &\approx -\alpha - (\kappa_s - \kappa_b)[\frac{\alpha}{\kappa_b} + \kappa_b R(1 + \cot^2(\kappa_b R))] \\ &= -\alpha - (\kappa_s - \kappa_b)[\frac{\alpha}{\kappa_b} + \kappa_b R(1 + \frac{\alpha^2}{\kappa_b{}^2})] \\ &\approx -\alpha - (\kappa_s - \kappa_b)\kappa_b R \end{aligned}$$

We also have

$$\kappa_s - \kappa_b = \frac{\kappa_s^{\ 2} - \kappa_b^{\ 2}}{\kappa_b + \kappa_b} \approx \frac{\kappa_s^{\ 2} - \kappa_b^{\ 2}}{2\kappa_b} = \frac{\alpha^2 + k^2}{2\kappa_b},$$

Since

$$\kappa_s \cot(\kappa_s R) = k\cot(kR + \delta_0)$$

we have

$$k\cot(kR + \delta_0) = -\alpha - \frac{1}{2}(\alpha^2 + k^2)R.$$

Suppose that $kR << 1$, then we have

$$k\cot\delta_0 = -\alpha - \frac{1}{2}k^2 R.$$

The parameter $k\cot\delta_0$ depends only on two parameters α and k. Then the total cross section is given by

$$\begin{aligned}\sigma &= \frac{4\pi}{k^2}\sin^2\delta_0 \\ &= \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0} \\ &= \frac{4\pi}{k^2+\alpha^2} \\ &= \frac{2\pi\hbar^2}{\mu}\frac{1}{E + \dfrac{\hbar^2\alpha^2}{2\mu}}\end{aligned}$$

which has a Breit-Wigner form.

19. Effective range approximation-II

The effective range approximation is useful for the S-wave scattering due to the short range potential.

(a) The bound state with $E_b = -\frac{\hbar^2}{2\mu}\alpha^2 < 0$

Here we consider the case when $\kappa_b R \approx \frac{\pi}{2}$, which is the condition for the existence of the bound state. We start with the equation

$$\kappa_b R\cot(\kappa_b R) = -\alpha R.$$

Since

$$-\cot(\kappa_b R) = -\tan(\frac{\pi}{2} - \kappa_b R) \approx -(\frac{\pi}{2} - \kappa_b R),$$

we get the relation

$$-(\frac{\pi}{2} - \kappa_b R) = \frac{\alpha R}{\kappa_b R}$$

or

$$\kappa_b R = \frac{\pi}{2} + \frac{\alpha}{\kappa_b},$$

where

$$\kappa_b{}^2 = -\alpha^2 + k_0{}^2.$$

Such a relation is known as *effective range relation*.

(b) Scattering state with $E_s = \dfrac{\hbar^2}{2\mu}k^2 > 0$

From the solution of the scattering problem, we have

$$\tan(kR + \delta_0) = \frac{kR}{\kappa_s R}\tan(\kappa_s R), \qquad \text{(from the boundary condition)}$$

and

$$R_{out}(r) = \frac{C}{r}\sin(kr + \delta_0). \qquad \text{for } r >> R.$$

Using the approximation

$$\frac{\tan(\kappa_s R)}{\kappa_s R} \approx \frac{\tan(\kappa_b R)}{\kappa_b R},$$

we have

$$\tan(kR+\delta_0)=\frac{kR}{\kappa_b R}\tan(\kappa_b R).$$

Then we get

$$k\tan(\kappa_b R)=\kappa_b\tan(kR+\delta_0)=\kappa_b\frac{\tan(kR)+\tan\delta_0}{1-\tan(kR)\tan\delta_0}.$$

Here we use the effective potential range;

$$\kappa_b{}^2=-\alpha^2+k_0{}^2\approx k_0{}^2\text{, or}\qquad \kappa_b\approx k_0.$$

Then we get

$$\kappa_b R=\frac{\pi}{2}+\frac{\alpha}{\kappa_b}\approx\frac{\pi}{2}+\frac{\alpha}{k_0}.$$

Thus we have

$$k\tan(\frac{\pi}{2}+\frac{\alpha}{k_0})=k_0\frac{kR+\tan\delta_0}{1-kR\tan\delta_0},$$

for $\tan(kR)\approx kR$ and $\kappa_b=k_0$. So we get

$$-k\cot(\frac{\alpha}{k_0})=-\frac{kk_0}{\alpha}=k_0\frac{kR+\tan\delta_0}{1-kR\tan\delta_0},$$

or

$$-\frac{k}{\alpha}=\frac{kR+\tan\delta_0}{1-kR\tan\delta_0},$$

or

$$(k^2R-\alpha)\tan\delta_0=k(1+\alpha R)$$

or

$$\cot\delta_0=\frac{(k^2R-\alpha)}{k(1+\alpha R)}=\frac{kR-\frac{\alpha}{k}}{1+\alpha R}$$

This can be written as

$$
\begin{aligned}
k\cot\delta_0 + \alpha &= \frac{k^2R-\alpha}{(1+\alpha R)} + \alpha \\
&= \frac{k^2R-\alpha+\alpha+\alpha^2R}{1+\alpha R} \\
&= \frac{(k^2+\alpha^2)R}{1+\alpha R} \\
&\approx (k^2+\alpha^2)R
\end{aligned}
$$

or

$$k\cot\delta_0 = -\alpha + (k^2+\alpha^2)R.$$

Note that the correct expression for $k\cot\delta_0$ is given by

$$k\cot\delta_0 = -\alpha + \frac{1}{2}(k^2+\alpha^2)R$$

for square-well potential (Bethe, Elementary Nuclear Physics). Thus the total scattering cross section is

$$
\begin{aligned}
\sigma_{tot} &= \frac{4\pi}{k^2}\sin^2\delta_0 \\
&= \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0} \\
&= \frac{4\pi}{k^2}\frac{k^2(1+R\alpha)^2}{(1+k^2R^2)(k^2+\alpha^2)} \\
&= \frac{4\pi(1+R\alpha)^2}{(k^2+\alpha^2)(1+k^2R^2)} \\
&\approx \frac{4\pi}{(k^2+\alpha^2)}
\end{aligned}
$$

Note that the total scattering cross section has a Breit-Wigner form. We define the scattering length as

$$\lim_{k\to 0} k\cot\delta_0 = -\alpha = -\frac{1}{a},$$

or

$$\alpha = \frac{1}{a}.$$

Then the total scattering cross section is

$$\sigma_{tot} = \frac{4\pi}{k^2 + \frac{1}{a^2}} = \frac{4\pi a^2}{1 + k^2 a^2}.$$

The scattering length can now be characterized by the fact that

$$\lim_{k \to 0} \sigma_{tot} = 4\pi a^2.$$

20. Effective potential with $l \neq 0$ and quasi bound state

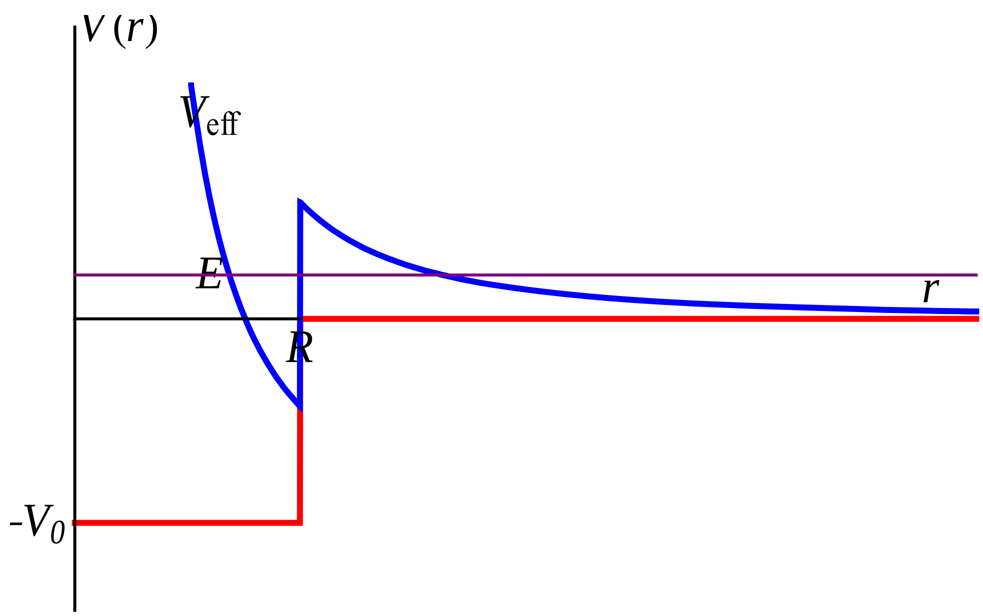
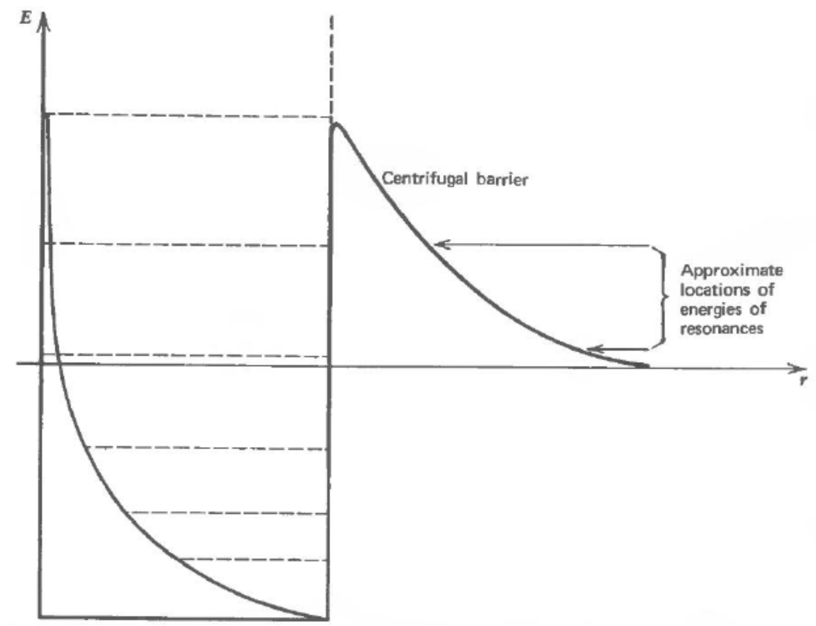


Fig. The centrifugal barrier combines with the potential well to form an effective potential, which can produce a metastable state.



The effective potential for the *l*-th partial wave ($l \neq 0$) is given by

$$V_{eff} = -V_0 + \frac{\hbar^2 l(l+1)}{2\mu r^2} \qquad (r<R)$$

where $V_0>0$ and μ is the reduced mass. As shown in the above figure, the effective potential has an attractive well followed by a repulsive barrier at larger distances. The particle can be trapped inside., but cannot be trapped forever. Such a trapped state has a finite lifetime as a consequence of quantum-mechanical tunneling. The particle leaks through the barrier to the outside region. Such a state is called a quasi-bound state.

((**Townsend**))

A particle with energy *E* greater than zero but less than the height of the barrier can tunnel through the barrier and form a metastable bound state in the wall. This state is metastable (and not stable) because a particle “trapped” inside the well can also tunnel out.

We consider the resonance scattering from a potential well

$$u''(r) + [k^2 - U(r) - \frac{l(l+1)}{r^2}]u(r) = 0, \qquad (1)$$

where

$$u(r) = rR(r).$$

For $r<R$

$$u''(r)+[-\alpha^2+U_0-\frac{l(l+1)}{r^2}]u(r)=0$$

with

$$E=-\frac{\hbar^2}{2m}\alpha^2$$

$$\kappa^2=-\alpha^2+U_0$$

$$R_{kl}(r)=\frac{u_{kl}(r)}{r}=Aj_l(\kappa r)$$

For $r>R$

$$u''(r)+(k^2-\frac{l(l+1)}{r^2})u(r)=0$$

$$R_{kl}(r)=\frac{u_{kl}(r)}{r}=Be^{i\delta_l}[\cos\delta_l j_l(kr)-\sin\delta_l n_l(kr)]$$

The continuity of $u_{kl}(r)$ and its derivative at $r = R$:

$$\begin{aligned}\frac{\kappa j_l'(\kappa R)}{j_l(\kappa R)}&=k\frac{[\cos\delta_l j_l'(kR)-\sin\delta_l n_l'(kR)]}{\cos\delta_l j_l(kR)-\sin\delta_l n_l(kR)}\\&=\frac{kj_l'(kR)-k\tan\delta_l n_l'(kR)}{j_l(kR)-\tan\delta_l n_l(kR)}\end{aligned}.$$

Thus we get

$$\tan\delta_l=\frac{kj_l'(kR)j_l(\kappa R)-\kappa j_l(kR)j_l'(\kappa R)}{kn_l'(kR)j_l(\kappa R)-\kappa n_l(kR)j_l'(\kappa R)}$$

For $x=kR<<l$, we use the approximation

$$j_l(x)\approx\frac{1}{1\cdot3\cdot5\cdot7\cdots(2l+1)}x^l$$

$$n_l(x)\approx1\cdot3\cdot5\cdot7\cdots(2l+1)x^{-(l+1)},$$

$$j_l'(x) \approx \frac{l}{1\cdot 3\cdot 5\cdot 7\cdots(2l+1)} x^{l-1}$$

$$n_l'(x) \approx 1\cdot 3\cdot 5\cdot 7\cdots(2l+1)(-l-1)x^{-(l+2)}$$

(i) Now we investigate the resonance scattering in detail for small energies and a very deep potential well;

$$kR << l << \kappa R.$$

$$\tan\delta_l = \frac{(2l+1)}{[(2l+1)!!]^2}(kR)^{2l+1} \frac{l - \kappa R \frac{j_l'(\kappa R)}{j_l(\kappa R)}}{l+1+\kappa R \frac{j_l'(\kappa R)}{j_l(\kappa R)}}$$

For $kR \to 0$, we have

$$\delta_l \approx (kR)^{2l+1}$$

The total cross section is

$$\sigma_l = \frac{4\pi}{k^2}\sin^2\delta_l \approx \frac{4\pi}{k^2}\delta_l^2 \approx \frac{1}{k^2}(kR)^{4l+2} \approx k^{4l}.$$

For sufficiently small energy, the partial waves with $l \geq 1$ therefore do not contribute.

(ii) We note that $\delta_l = \frac{\pi}{2}$, when

$$kn_l'(kR)j_l(\kappa R) - \kappa n_l(kR)j_l'(\kappa R) = 0.$$

Then we have

$$(l+1)k(kR)^{-1} j_l(\kappa R) + \kappa j_l'(\kappa R) = 0$$

or

$$l+1+\kappa R\frac{j_l'(\kappa R)}{j_l(\kappa R)} = 0.$$

Using the asymptotic form

$$j_l(x) \approx \frac{1}{x}\sin(x-\frac{\pi}{2}l)\,, \qquad j_l'(x) \approx \frac{1}{x}\cos(x-\frac{\pi}{2}l)\,,$$

$$n_l(x) \approx -\frac{1}{x}\cos(x-\frac{\pi}{2}l)\,, \qquad n_l'(x) \approx \frac{1}{x}\sin(x-\frac{\pi}{2}l)\,.$$

So we have

$$\frac{l+1}{R}\sin(\kappa R-\frac{\pi}{2}l)+\kappa\cos(\kappa R-\frac{\pi}{2}l)=0\,,$$

or

$$\cot(\kappa R-\frac{\pi}{2}l)=-\frac{l+1}{\kappa R}\,,$$

or

$$\tan(\kappa R-\frac{\pi}{2}l-\frac{\pi}{2})=\frac{l+1}{\kappa R}\,.$$

Since the right hand side is very small, we get

$$\kappa R-\frac{l\pi}{2}\approx(n+\frac{1}{2})\pi+\frac{l}{\kappa R}.$$

where n is an positive integer. The resonant scattering occurs when the incident energy is just such as to match an energy level.

20. Connection between resonance and binding energy

(a) S-matrix element for the low-energy scattering

We start with

$$\kappa_s\cot(\kappa_s R)=k\cot(kR+\delta_0)$$

for the low-energy S-wave scattering, where

$$\kappa_s{}^2R^2=k^2R^2+k_0{}^2R^2\,.$$

Here we determine the S-matrix element

$$S=e^{2i\delta_0}\,.$$

using the formula

$$\cot x = i\frac{e^{2ix}+1}{e^{2ix}-1}.$$

Thus we get

$$S = e^{2i\delta_0} = e^{-2ikR}\frac{\cos(\kappa_s R) + i\frac{k}{\kappa}\sin(\kappa_s R)}{\cos(\kappa_s R) - i\frac{k}{\kappa}\sin(\kappa_s R)}$$

As is expected, the expression for S has unit modulus. There is a remarkable relation between the S-matrix and bound states. We set

$$k \to i\alpha, \qquad \kappa_s \to \kappa_b$$

Then the function S has a pole for

$$\cos(\kappa_b R) + \frac{\alpha}{\kappa_b}\sin(\kappa_b R) = 0$$

or

$$\kappa_b \cot(\kappa_b R) = -\alpha$$

which is exactly the same expression derived from the approach from the wave function of the bound state. In general, the poles of $S_l(k)$ for $k = i\alpha$ give the position of the bound states in the l-th partial wave.

(b) Approach form the binding energy

Using the Taylor expansion, we expand the quantity

$$\kappa_s \cot(\kappa_s R),$$

around $\kappa = \kappa_b$, where

$$\kappa_b \cot(\kappa_b R) = -\alpha.$$

We have

$$\kappa_s \cot(\kappa_s R) = \kappa_b \cot(\kappa_b R) + [\cot(\kappa_b R) - \kappa_b R \csc^2(\kappa_b R)](\kappa_s - \kappa_b) + ...$$
$$\approx -\alpha - (\kappa_s - \kappa_b)[\frac{\alpha}{\kappa_b} + \kappa_b R(1 + \cot^2(\kappa_b R)]$$
$$= -\alpha - (\kappa_s - \kappa_b)[\frac{\alpha}{\kappa_b} + \kappa_b R(1 + \frac{\alpha^2}{\kappa_b{}^2})]$$
$$\approx -\alpha - (\kappa_s - \kappa_b)\kappa_b R$$

We also have

$$\kappa_s - \kappa_b = \frac{\kappa_s{}^2 - \kappa_b{}^2}{\kappa_s + \kappa_b} \approx \frac{\kappa_s{}^2 - \kappa_b{}^2}{2\kappa_b},$$

We note that

$$\kappa_b \cot(\kappa_b R) = -\alpha,$$

$$\kappa_b{}^2 = -\alpha^2 + k_0{}^2,$$

$$\kappa_s{}^2 = k^2 + k_0{}^2,$$

and

$$U_0 = \frac{2m}{\hbar^2} V_0 = k_0{}^2.$$

Finally we have

$$\kappa_s \cot(\kappa_s R) = -\alpha - (\kappa_s - \kappa_b)\kappa_b R$$
$$\approx -\alpha - (\frac{\kappa_s{}^2 - \kappa_b{}^2}{2\kappa_g})\kappa_g R$$
$$= -\alpha - (\frac{\kappa_s{}^2 - \kappa_b{}^2}{2})R$$
$$\approx -\alpha - \frac{(\kappa_s{}^2 + \alpha^2 - k_0{}^2)}{2} R$$
$$\approx -\alpha - \left(\frac{k^2 + \alpha^2}{2}\right)R$$

or

$$\kappa_s \cot(\kappa_s R) = -\alpha - \left(\frac{k^2 + \alpha^2}{2}\right) R .$$

(c) Approach from the S-wave scattering

We also note that

$$\tan(kR + \delta_0) = \frac{kR}{\kappa_s R} \tan(\kappa_s R) ,$$

or

$$\frac{\tan(kR)\cot\delta_0 + 1}{\cot\delta_0 - \tan(kR)} = \frac{k}{\kappa_s \cot(\kappa_s R)} ,$$

or

$$\kappa_s \cot(\kappa_s R) = \frac{k\cot\delta_0 - k\tan(kR)}{\tan(kR)\cot\delta_0 + 1} \approx \frac{k\cot\delta_0 - k^2 R}{kR\cot\delta_0 + 1} ,$$

or

$$\begin{aligned}
\kappa_s \cot(\kappa_s R) - k\cot\delta_0 &= \frac{k\cot\delta_0 - k^2 R}{kR\cot\delta_0 + 1} - k\cot\delta_0 \\
&= \frac{k\cot\delta_0 - k^2 R - k\cot\delta_0 (kR\cot\delta_0 + 1)}{kR\cot\delta_0 + 1} \\
&= \frac{-(k^2 + k^2\cot^2\delta_0)}{kR\cot\delta_0 + 1} R \\
&\approx -(k^2 + k^2\cot^2\delta_0) R \\
&\approx -(k^2 + \alpha^2) R
\end{aligned}$$

or

$$\kappa_s \cot(\kappa_s R) = k\cot\delta_0 - (k^2 + \alpha^2) R .$$

Here we note that

$$k\cot\delta_0 = \frac{(k^2 R - \alpha)}{k(1 + \alpha R)} = \frac{k^2 R - \alpha}{1 + \alpha R} \approx -\alpha .$$

(d) Effective range and scattering length

From two expressions of $\kappa_s \cot(\kappa_s R)$ shown above, we get

$$\kappa_s \cot(\kappa_s R) = k\cot\delta_0 - (k^2+\alpha^2)R = -\alpha - \frac{(k^2+\alpha^2)}{2}R$$

Then we have

$$k\cot\delta_0 = -\alpha + \frac{(k^2+\alpha^2)}{2}R$$ (the effective range expansion)

The scattering length *a* is defined by

$$\lim_{k\to 0} k\cot\delta_0 = \lim_{k\to 0}(-\alpha + \frac{k^2+\alpha^2}{2}R) = -\alpha + \frac{\alpha^2}{2}R \approx -\alpha = -\frac{1}{a}$$

or

$$\frac{1}{a} = \alpha.$$

((**Note**))

In the early days of nuclear physics, many attempts were made to fit experimental data on low–energy scattering phase shifts for the nucleon-nucleon system. It was found that there was a peculiar insensitivity to the precise potential shape and the data could be fit by almost any shape. The essential result was that the function $k\cot\delta_0$ is to excellent approximation a linear function of k^2,

$$k\cot\delta_0 = -\alpha - \frac{1}{2}(k^2+\alpha^2)R,$$

The parameters *a* is called the scattering length, whereas *R* is called the effective range, and the approximation is referred to as the effective-range approximation.

Using this scattering length, the total cross section can be rewritten as

$$\begin{aligned}\sigma_{tot} &= \frac{4\pi}{k^2}\frac{1}{1+\cot^2\delta_0} \\ &= \frac{4\pi}{k^2 + k^2\cot^2\delta_0} \\ &= \frac{4\pi}{k^2 + \frac{1}{a^2}} \\ &= \frac{4\pi a^2}{1+a^2k^2}\end{aligned}$$

The low-energy form of the scattering amplitude is given by

$$\begin{aligned}f(k) &= \frac{1}{k}e^{i\delta_0}\sin\delta_0 \\ &= \frac{1}{k}\sin\delta_0(\cos\delta_0 + i\sin\delta_0) \\ &= \frac{1}{k}\sin\delta_0\frac{(\cos\delta_0 + i\sin\delta_0)(\cos\delta_0 - i\sin\delta_0)}{(\cos\delta_0 - i\sin\delta_0)} \\ &= \frac{1}{k\cot\delta_0 - ki} \\ &= \frac{-a}{1+ika} \\ &= \frac{-i}{k-\frac{i}{a}}\end{aligned},$$

using the effective-range approximation. Then $f(k)$ has a simple pole at

$$k = \frac{i}{a} = i\alpha$$

We note that in the low energy limit the optical theorem

$$\begin{aligned}\sigma_{tot} &= \frac{4\pi}{k}\mathrm{Im}[f(k)] \\ &= \frac{4\pi}{k}\mathrm{Im}[-\frac{a}{1+ika}] \\ &= \frac{4\pi}{k}\mathrm{Im}[-\frac{a(1-ika)}{1+k^2a^2}] \\ &= 4\pi a^2\frac{1}{1+k^2a^2} \approx 4\pi a^2\end{aligned}$$

((**Note**)) Deuteron as an example

$s = 1 \quad {}^3S_1$

((Definition of the scattering length α))

$$\lim_{k\to 0} k\cot\delta_0 = \lim_{k\to 0}(-\alpha + \frac{k^2+\alpha^2}{2}R) = -\alpha + \frac{\alpha^2}{2}R = -\frac{1}{a}$$

or

$$\frac{1}{a} = \alpha - \frac{\alpha^2}{2}R. \qquad (1)$$

In the spin triplet channel, the scattering length a and effective range R are

a = 5.42 fm, R = 1.75 fm,

respectively, while the binding energy is 2.23 MeV. This means that

$$|E_b| = \frac{\hbar^2}{2\mu}\alpha^2 = 2.23 \text{ MeV}, \qquad \alpha = 0.232 \text{ fm}^{-1}.$$

where

$$\mu = \frac{m_p m_n}{m_p + m_n} = 8.36887 \times 10^{-25} \text{ g}$$

With these values both sides of Eq.(1) have the value 0.185 fm^{-1};

$$\frac{1}{a} = 0.1845 \text{ fm}^{-1},$$

$$\alpha - \frac{\alpha^2}{2}R = 0.1848 \text{ fm}^{-1}.$$

21. Breit-Wigner resonance formula

The cross section for pure elastic scattering for the l-th partial wave is

$$\sigma_{el}^{l} = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$$
$$= \frac{4\pi}{k^2}(2l+1)\frac{1}{1+\cot^2\delta_0}$$

This has a maximum when $\delta_l(E_0) = \frac{\pi}{2}$ at $E = E_0$.

$$\delta_l(E_0) = \frac{\pi}{2}$$

We expand $\cot[\delta_l(E)]$ around $E = E_0$ using the Taylor expansion as

$$\cot[\delta_l(E)] = \cot[\delta_l(E_0)] + \left(\frac{d}{dE}\cot\delta_l\right)_{E=E_0}(E-E_0) + ...$$
$$= -\left(\frac{1}{\sin^2\delta_l}\frac{d\delta_l}{dE}\right)_{E=E_0}(E-E_0) + ...$$

Here we define

$$\left(\frac{d\delta_l}{dE}\right)_{E=E_0} = \frac{2}{\Gamma}.$$

Then we get

$$\cot[\delta_l(E)] = -\frac{2}{\Gamma}(E-E_0) + ...$$

$$f(\theta) = \sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta),$$

with

$$
\begin{aligned}
f_l(k) &= \frac{1}{k} e^{i\delta_l} \sin(\delta_l) \\
&= \frac{1}{k} \frac{\sin(\delta_l)}{\cos(\delta_l) - i\sin(\delta_l)} \\
&= -\frac{1}{k} \frac{1}{\frac{2}{\Gamma}(E - E_0) + i} \quad , \\
&= -\frac{1}{k} \frac{\frac{\Gamma}{2}}{(E - E_0) + i\frac{\Gamma}{2}}
\end{aligned}
$$

The total cross section is

$$
\begin{aligned}
\sigma_l &= \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l \\
&= \frac{4\pi}{k^2}(2l+1)\frac{1}{1+\cot^2\delta_l} \\
&= \frac{4\pi}{k^2}(2l+1)\frac{\frac{\Gamma^2}{4}}{\frac{\Gamma^2}{4} + (E - E_0)^2}
\end{aligned}
$$

The factor

$$
P(E) = \frac{\frac{\Gamma^2}{4}}{\frac{\Gamma^2}{4} + (E - E_0)^2},
$$

is called as a *Breit-Wigner factor*.

22. Definition of scattering length *a*

In the limit of $k \to 0$,

$$
\begin{aligned}
u_{out}(r) &= rR_{out}(r) \\
&= C\cos\delta_0[\sin(kr) + \cos(kr)\tan\delta_0] \\
&\approx C'(r + \lim_{k\to 0}\frac{\tan\delta_0}{k}) \\
&= C'(r - a)
\end{aligned}
$$

Here we define the scattering length a as

$$a = -\lim_{k \to 0} \frac{\tan \delta_0}{k}.$$

or

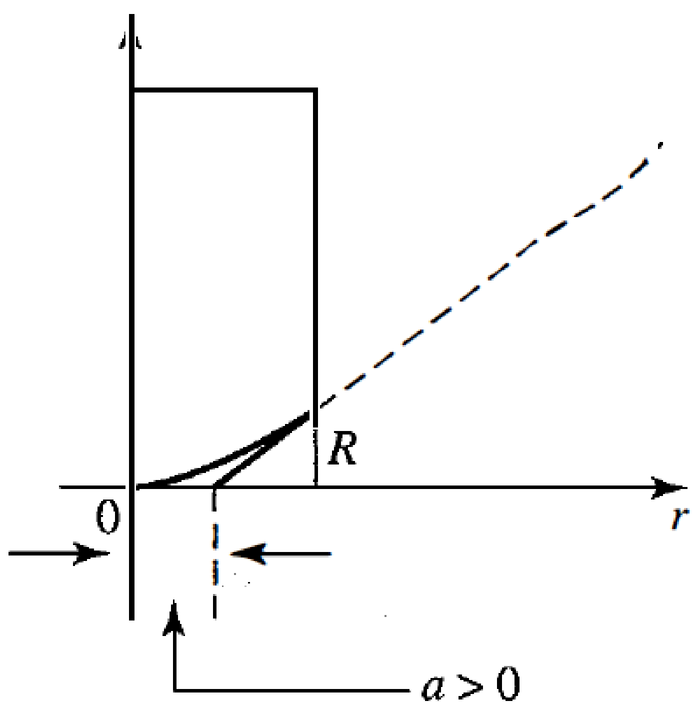
$$\lim_{k \to 0} k \cot \delta_0 = -\frac{1}{a}.$$

Thus we have the wave function as

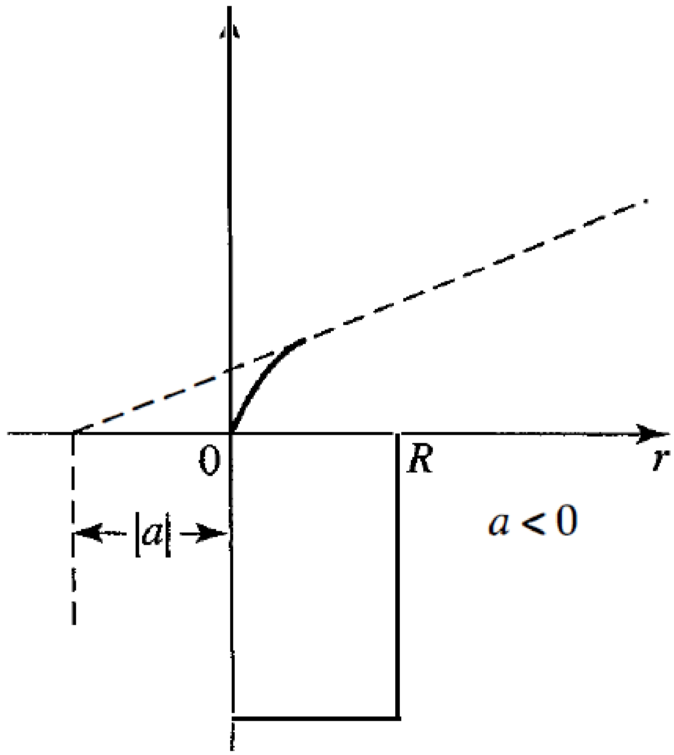
$$u_{out}(r) = C'(r - a).$$

The total cross section in the limit of $k \to 0$ is given by

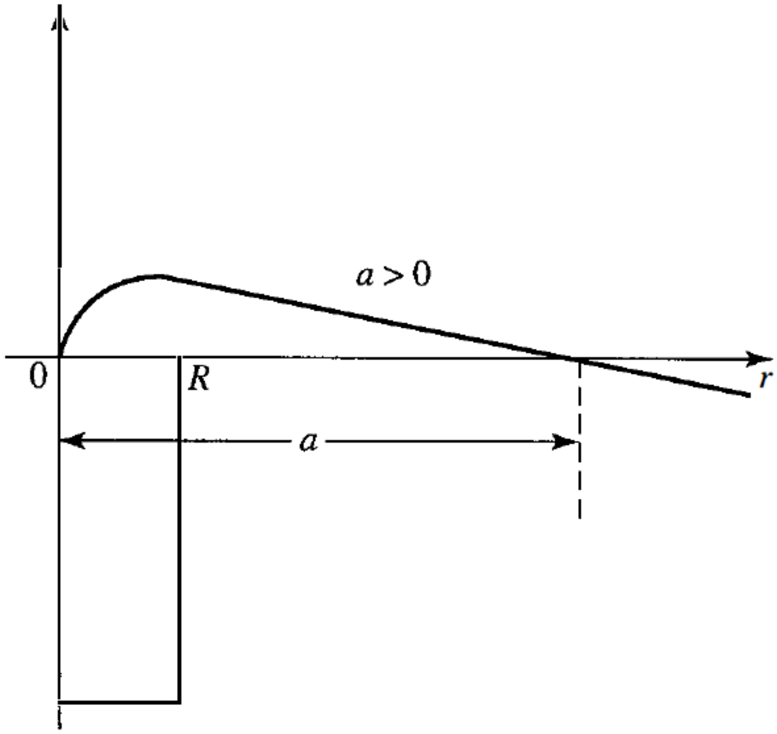
$$\sigma_{tot} = \frac{4\pi}{k^2} \sin^2 \delta_0 = 4\pi \lim_{k \to 0} \left| \frac{1}{k \cot \delta_0 - ik} \right| = 4\pi a^2.$$



(a) Repulsive potential. The scattering length a is positive (a>0). For the infinite potential height, the scattering length a is equal to R, since $u(r = R) = 0$.



(b) Attractive potential without a bound state. The scattering length a is negative ($a<0$). $u(r=0) = 0$.



(c) Deeper attractive potential with a single bound state. *a* is the scattering length. *a*>0. . *u*(*r*=0) = 0.

23. Levinson's theorem

The Levinson's theorem relates the phase shift as zero and infinite energy to the number of bound states.

There is a remarkable theorem due to Norman Levinson, which relates the behavior of the phase shift for *E*>0 to the number of bound states with *E*<0. We already show that the number of bound states as a function of κR is closely related to that of the phase shift as a function of κR.

(i) $0 < \kappa R < \frac{\pi}{2}$ $\delta = 0$

There is no bound state

(ii) $\frac{\pi}{2} < \kappa R < \frac{3\pi}{2}$ $\delta = 1\pi$

There is one bound state

(iii) $\frac{3\pi}{2} < \kappa R < \frac{5\pi}{2}$ $\delta = 2\pi$

There is two bound states

(iv) $\frac{5\pi}{2} < \kappa R < \frac{7\pi}{2}$ $\delta = 3\pi$

There is three bound states.

In other words, we have the relation

$$\delta = N\pi$$

where N is the number of bound states. This relation is called the Levinson's theorem. In general we have

$$\delta_l = N_l \pi$$

for any l.

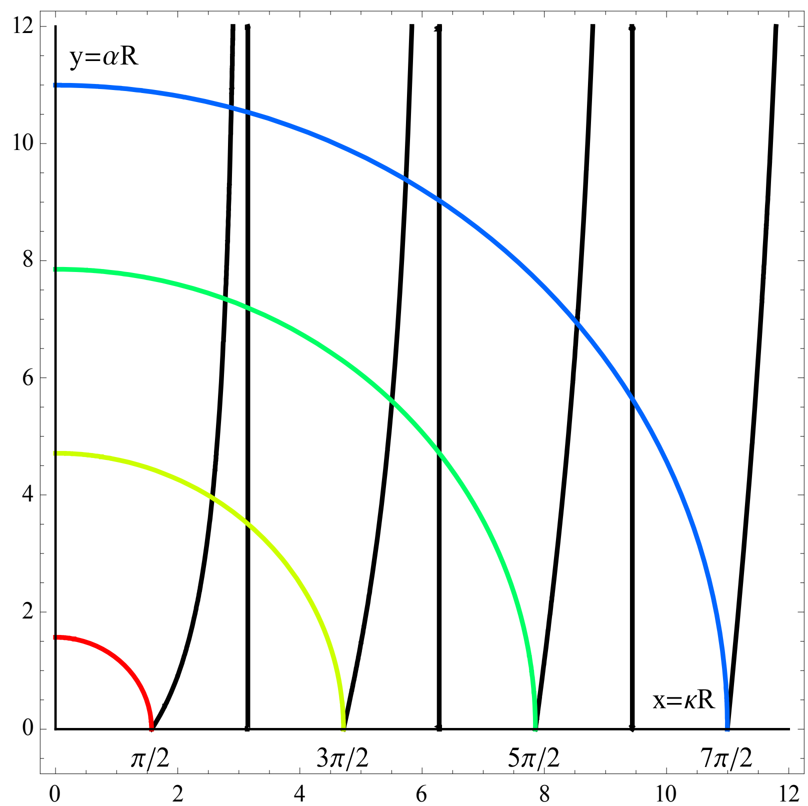


Fig. Graphical solution for the number of bound states.

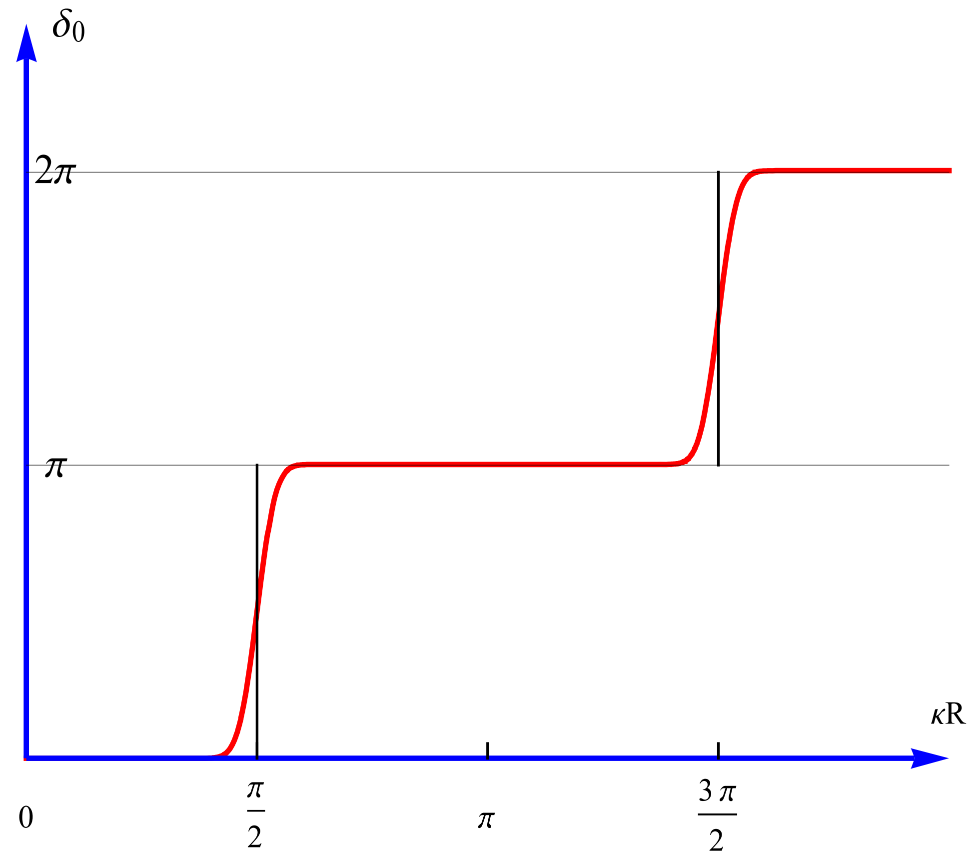
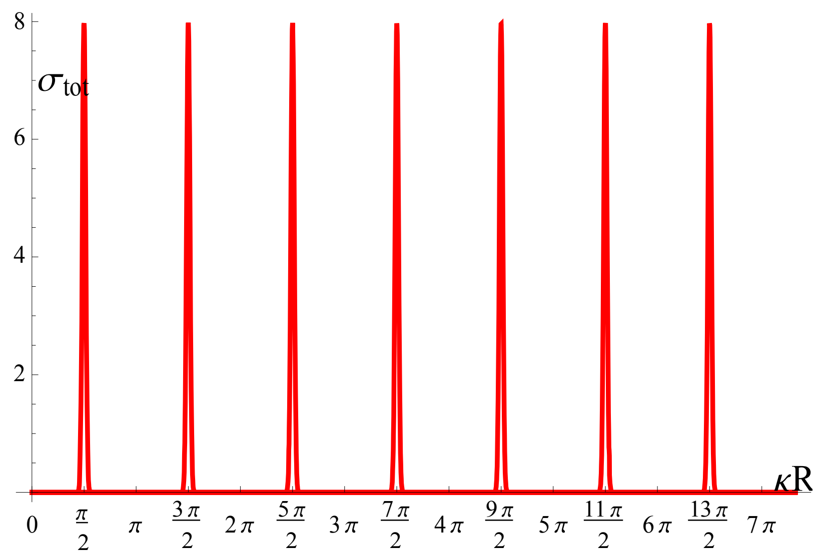


Fig. Schematic diagram for the phase shift vs κR.

24. How to determine the depth of the square-well potential.



$$(\kappa R)^2 = (kR)^2 + (k_0 R)^2$$

and

$$U_0 = \frac{2m}{\hbar^2} V_0 = k_0{}^2$$

Suppose that κR is a littler smaller than $\frac{2n+1}{2}\pi$. We slightly increase $(kR)^2$ (which is proportional to the kinetic energy). When

$$\kappa R = \frac{2n+1}{2}\pi$$

the total cross section increases drastically. Since $kR << 1$, we can evaluate the depth of the potential as

$$k_0 R = \sqrt{\frac{2m}{\hbar^2} V_0} R = \frac{2n+1}{2}\pi \ .$$

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APPENDIX What the Ramsauer-Townsend effect meant for Bohr in 1920's

Before I read the book of H. Kragh, I do not understand why this effect is so often discussed in the scattering in the quantum mechanics. But after I read the book, I realized that this effect is very important as well as the Frank-Hetz experiment. The Ramsuaer effect is the phenomenon of elastic scattering for electrons, while the Frank-Hertz experiment is the phenomenon of inelastic scattering for electrons. Here I put the following sentences in the book written by H. Kragh.

H. Kragh, Niels Bohr and the Quantum Atom: The Bohr Model of Atomic Structure 1913-1925 (Oxford, 2012) p.261.

((**Kragh**))

There were other anomalies that played a similarly minor role in the crisis that eventually led to the fall of the Bohr–Sommerfeld theory. One of them was the Ramsauer effect, so named after the Heidelberg physicist Carl Ramsauer who, at a meeting of German scientists in Jena in September 1921, reported some startling results concerning the penetrability of slow electrons in an argon gas. A few earlier physicists had observed that slow cathode rays move more freely through a gas than fast ones, but it was only with Ramsauer's work that the effect became generally known and aroused widespread attention in the physics community. Franck (James Franck, nown as the Frank-Hertz experiment), who had participated in the Jena meeting, reported to Bohr: 'In Jena I was particularly interested in a paper of Ramsauer that I am not able to believe, though I cannot show any mistake in the experiment. Ramsauer obtained the result that in argon the free path lengths are tremendously large at very low velocity of electrons. If this result is right, it seems to me fundamental. Bohr replied that he was very interested in the new result and wanted more information about it. He thought that the question was probably 'very closely connected with the general views of atomic structure. Franck and Bohr were not the only physicists who found Ramsauer's experiments puzzling. In November Born wrote to Einstein about 'Ramsauer's quite crazy assertion (in Jena) that in argon the path length of the electrons tends to infinity with decreasing velocity (slow electrons pass freely through atoms!)'. He added that 'This we would like to refute!' The initial skepticism with regard to the Ramsauer effect evaporated after it was confirmed by experiments carried out by, among others, Gustav Hertz in Eindhoven, Hans Mayer in Heidelberg, and Rudolph Minkowski and Hertha Sponer in Göttingen. Not only was the effect real, it also turned out that it was not limited to argon but appeared in the other noble gases as well and possibly was a general property of matter in the gaseous state. The phenomenon defied theoretical explanation, whether in terms of classical theory or quantum theory. The first to take up the challenge was young Friedrich Hund, who at the time was a doctoral student under Born in Göttingen. Inspired by Franck, he developed a theory based on quantum conditions and the correspondence principle, from which followed that slow electrons would not be influenced by collisions with gas molecules.126 Bohr was keenly interested in Hund's theory, which he knew in outline from his correspondence with Franck. Although the theory was somewhat unorthodox, he thought it agreed with the spirit of quantum theory. 'I see no other simple explanation of the Ramsauer experiment', he wrote to Franck, 'and am so skeptical about the established principles of physics that I do not feel justified in rejecting your [and Hund's] ideas as total nonsense'.127 However, Hund's theory turned out to be untenable and it was not replaced by better theories. The Ramsauer effect thus remained unexplained, without the lack of explanation causing much concern at the time. Although physicists in Copenhagen and Göttingen were convinced that it was a quantum effect, other physicists thought of it in terms of classical gas theory or simply avoided attempts of explanation. At any rate, by far the most work on the Ramsauer effect was experimental, an autonomous line of research that was uninfluenced by quantum theory. The Ramsauer effect was anomalous, but it was not obvious that the anomaly belonged to the domain of quantum theory. This may explain the limited role it played during the last years of the old quantum theory, when it was no more significant than the Paschen–Back effect. It is noteworthy that the Ramsauer anomaly did not appear in any of the editions of Sommerfeld's *Atombau* or in Born's *Atommechanik*. It only received a partial explanation in 1925, when Walter Elsasser used Louis de Broglie's new ideas of matter-waves to explain how slow electrons can penetrate almost freely through gases because of their very large wavelength (as given by the de Broglie formula $\lambda = h/mv$).128 At about the same time Bohr returned to the effect and how to understand it in a broader physical context. He revealed some of his thoughts in a letter to Geiger of April 1925. Recently I have also felt that an explanation of collision phenomena, especially Ramsauer's results on the penetration of slow electrons through atoms, presents difficulties to our ordinary space-time description of nature similar in kind to those presented by the simultaneous understanding of interference phenomena and a coupling of changes of state of separated atoms by radiation. I believe that these difficulties exclude the retention of the ordinary space-time description of phenomena to such an extent that, in spite of the existence of coupling, conclusions about a possible corpuscular nature of radiation lack a sufficient basis.