18. Hard Sphere, Step Barrier, and Square Well Potentials

For these simple potentials, the scattering problem can be solved in closed form, in both the semiclassical and quantum treatments. The notation we shall use is defined in Fig. 18-1.

**Hard Sphere**

\[ V(r) = \begin{cases} \infty, & r < \sigma \\ 0, & r \geq \sigma \end{cases} \]

\[ A = \frac{\mu n \sigma}{\hbar} = \left(\frac{2\mu E}{\hbar^2} \sigma^2\right)^{1/2} \]

\[ B = 2\mu \sigma^2 / \hbar^2 \]

\[ \beta = b / \sigma \]

**Step Barrier**

\[ V(r) = \begin{cases} \infty, & r < \sigma \\ 0, & r \geq \sigma \end{cases} \]

**Square Well**

\[ V(r) = \begin{cases} \infty, & r < \sigma \\ 0, & r \geq \sigma \end{cases} \]

Fig. 18-1

For all three potentials, the semiclassical phase shift, deflection angle, and collision lifetime vanish unless \( b < \sigma \), as is obvious from the formulas of Table 5-1.

In the hard sphere case, \( r_c = \sigma \) (when \( b < \sigma \)) and the formulas given in Table 5-1 reduce to

\[ n = -\frac{1}{A} \left[ \left( 1 - \frac{b^2}{r^2} \right)^{1/2} \right]^{1/2} \]

\[ dr = -A[1 - \beta^2]^{1/2} - \beta \arccos(\beta) \]  

(18-1)
\[ \chi = 2b \int_{b}^{r} \left( 1 - \frac{b^2}{r^2} \right)^{-1/2} r^{-2} dr = 2\arccos \beta \]  

(18-2)

\[ \tau = -\frac{2}{\sqrt{\nu}} \int_{b}^{r} \left( 1 - \frac{b^2}{r^2} \right)^{-1/2} dr = -\frac{2\sqrt{\nu}}{1 - \beta^2} \]  

(18-3)

In terms of the dimensionless reduced variables \( A \) and \( \beta \), the derivative relations given in Table 5.1 become

\[ \chi = \frac{2}{A} \frac{(\partial \eta)}{\partial \beta} \]  

(18-4)

\[ \tau = \frac{K}{E} \left[ \frac{(\partial \eta)}{\partial \beta} - \beta \frac{(\partial \eta)}{\partial \beta} \right] \]  

(18-5)

and these are readily verified. Graphs of \( \eta \), \( \chi \), and \( \tau \) as functions of the reduced impact parameter \( \beta \) are shown in Fig. 18-2. Note that \( \eta(\beta) \) is simply proportional to velocity, \( \chi(\beta) \) is independent of velocity, and \( \tau(\beta) \) is inversely proportional to velocity.
The classical differential and total cross sections for hard sphere scattering are given by

\[ I(\chi) = \sigma^2 \left| \sin \chi \right|^{\alpha} \left( \frac{\sin \chi}{\chi} \right)^{-1} = \frac{1}{\alpha^2} \sigma^2 \]  

(18-6)

\[ \sigma = 2\pi \int_0^\infty I(\chi) \sin \chi \, d\chi = \pi \sigma^2 \]  

(18-7)

Thus, as expected, the scattering is isotropic and the total cross section is simply the geometrical cross section. The formula for \( \chi(b) \) also has a simple intuitive interpretation, as indicated in Fig. 18-3; it corresponds to specular reflection of the incident beam from the surface of the sphere

\[ \chi = 0, \quad b > \sigma \]

\[ \chi = 2\alpha \]

\[ = 2 \arccos \frac{b}{\sigma}, \quad b < \sigma \]

Fig. 18-3

The exact quantum partial wave treatment of hard sphere scattering has been discussed in some detail by Massey and Mohr. They show that the phase shifts are given by

\[ \sin^2 \eta^m_2 = \frac{J^2_m(A)}{J^2_m(A) + N^2_m(A)}, \]  

(18-8)
where \( m = \Re + \frac{1}{2} \) and \( J \) and \( M \) are the Bessel functions of the first and second kind.

For the square well potential, the turning radius and impact parameter are related by

\[
r_c = \frac{b}{n},
\]

(18-9)

where we define the index of refraction of the well by

\[
n = \sqrt{1 + \frac{\beta}{E}} ^{1/2} > 1.
\]

(18-10)

In this case the semiclassical formulas of Table 5-1 reduce to the hard sphere results of Eqs. (18-1) to (18-3) plus a term of the same functional form but of opposite sign and with \( \beta = \beta/n, A = nA \). To show how this comes about, we shall evaluate the phase function,

\[
\eta = \frac{1}{2\pi} \left\{ \int_{r_c}^{\infty} \left[ 1 - \frac{b^2}{r^2} + \frac{V(r)}{E} \right]^{1/2} dr - \int_{b}^{\infty} \left[ 1 - \frac{b^2}{r^2} \right]^{1/2} dr \right\},
\]

which becomes, for the square well potential,

\[
\eta = \frac{1}{2\pi} \left\{ \int_{b/n}^{\infty} \left[ 1 - \frac{b^2}{r^2} \right]^{1/2} dr - \int_{b}^{\infty} \left[ 1 - \frac{b^2}{r^2} \right]^{1/2} dr \right\}.
\]

In terms of the dimensionless variables \( x = r/\sigma, \beta = b/\sigma, A = \sigma/\lambda \), this is

\[
\eta = \frac{1}{2\pi} \left\{ \int_{b/n}^{\infty} \left[ 1 - \frac{\beta^2}{x^2} \right]^{1/2} dx - \int_{\beta}^{\infty} \left[ 1 - \frac{\beta^2}{x^2} \right]^{1/2} dx \right\},
\]

which has the stated form. As illustrated later, the second integral, independent of \( n \), represents "edge scattering". Thus the phase shift, deflection angle, and delay time functions are given by

\[
\eta = \frac{1}{2\pi} \ln \left( \frac{1}{n \left( 1 - \frac{\beta^2}{n^2} \right)} \right) - \frac{1}{n} \left( \frac{1}{\beta^2} - \frac{1}{\sigma} \right) - \frac{1}{\beta} (\arccos \beta - \arccos \frac{\beta}{n})
\]

(18-11)
\[ \chi = -2 \left[ \arccos \frac{\beta}{\sqrt{n}} - \arccos \beta \right] \]  

(18-12)

\[ \tau = \frac{2\sigma}{\sqrt{n}} \left[ \frac{1}{n} \left( \frac{1}{2} - \frac{\beta^2}{2} \right)^{1/2} - \left( \frac{1}{2} - \beta^2 \right)^{1/2} \right] \]  

(18-13)

In \( \eta \) and \( \chi \) the term involving \( n \) is dominant, the more so the larger \( n \), so that the signs are opposite to those for hard sphere scattering, as would be expected for any purely attractive potential. For \( n \to 1 \), everything vanishes, of course, as then there is no potential. In the limit \( n \to \infty \), corresponding to an infinitely deep well, \( \eta \) increases without limit, whereas

\[ \chi \to -\pi + 2\arccos \beta, \]  

(18-14)

that is, the deflection exhibits the same "edge scattering" as the hard sphere case, plus a negative "interior deflection" which can become as large as \(-\pi\) for \( n \to \infty \).

The analogy with refraction of light by a sphere is indicated in Fig. 18-4.

Here we have

\[ \alpha = \alpha' + \beta \] and \( \chi = -\chi/2 \)

\[ \sin \alpha = b/\sigma = \beta \]

\[ \sin \alpha' = \frac{1}{n} \sin \alpha. \]
Thus

\[ \chi = \frac{\chi}{2} = \arcsin\beta - \arcsin\frac{\beta}{n} \]

\[ = \arccos\frac{\beta}{n} - \arccos\beta, \]

in agreement with (18-12). Incidentally, we should note that in terms of velocities "inside" and "outside" the index of refraction has a different interpretation for particles than for light. The light ray is slowed down as it enters the sphere (velocity ratio \( v_i/v_0 = 1/n \) at edge of the sphere), whereas a particle beam is accelerated (velocity ratio \( v_i/v_0 = n \) at the edge).

Fig. 18-5 shows a graph of \( \chi(\beta) \) for several values of the index of refraction.

![Graph showing \( \chi(\beta) \) for several values of n.

Fig. 18-5

It is convenient to obtain an explicit expression for \( \beta(\chi, n) \) to use in evaluating the differential cross section. From (18-12),

\[ \arcsin\frac{\beta}{n} = \arcsin\beta + \frac{\chi}{2}, \]

Thus

\[ \frac{\beta}{n} = \beta\cos\frac{\chi}{2} + \left(1 - \beta^2\right)^{1/2} \sin\frac{\chi}{2}, \]

or
\[ n^2 \left( \frac{1}{n} - \cos \frac{\chi}{2} \right)^2 = (1 - \beta^2)^{1/2} \sin^2 \frac{\chi}{2} \]

and

\[ \beta^2 = \frac{n^2 \sin^2 \frac{\chi}{2}}{1 + n^2 - 2n \cos \frac{\chi}{2}} \]  \hspace{1cm} (18-15)

The cross section is given by

\[ I(\chi) = \frac{1}{2} \sigma^2 \left| \sin \left( \frac{\delta \chi}{2} \beta^2 \right) \right|^{-1} = \frac{n^2 \sigma^2}{4 \cos^2 \frac{\chi}{2}} \frac{(n \cos \frac{\chi}{2} - 1)(n - \cos \frac{\chi}{2})}{(1 + n^2 - 2n \cos \frac{\chi}{2})} \]  \hspace{1cm} (18-16)

Note that

\[ I(\chi = 0) = \sigma^2 n^2 / 4. \]

Fig. 18-6 gives the angular distribution for several values of \( n \). The special case where \( E = \epsilon \) corresponds to \( n = \sqrt{2} \).

![Graph showing angular distribution for different values of \( n \).]

Another simple potential may be synthesized by combining the square well with the hard sphere, so that
\[ V(r) = 0, \quad \sigma < r \]
\[ = -\varepsilon, \quad \rho \leq r \leq \sigma \]
\[ = \infty, \quad r < \rho. \]

In this case, the turning points are given by
\[ r_c = \rho, \] for \( 0 \leq b \leq n\rho \)
\[ = b/n, \] for \( n\rho \leq b \leq \sigma \)
\[ = b, \] for \( \sigma < b. \)

The results will be identical to those for a square well, with the addition of extra hard sphere terms for the \( 0 \leq b \leq n\rho \) range which are appropriate to the repulsive core of radius \( \rho. \) Thus, if we write \( \theta' = b/\rho = \theta(\sigma/\rho), \) then the terms to be added when \( 0 < \theta' < n \) are

\[ n = -A \frac{\rho}{\sigma} \left[ n \left( 1 - \frac{\theta'^{2}}{n^{2}} \right)^{1/2} + \theta' \arccos \frac{\theta'}{n} \right] \]  
(18-17)

\[ \chi = 2 \arccos \frac{\theta'}{n} \]  
(18-18)

\[ \tau = -\frac{2\rho}{v} \frac{1}{n} \left( 1 - \frac{\theta'^{2}}{n^{2}} \right)^{1/2} \]  
(18-19)

For example, consider the deflection angle,

\[ \chi = -2b \int_{r_c}^{\infty} \left[ 1 - \frac{b^{2}}{r^{2}} - \frac{V(r)}{\varepsilon} \right]^{-1/2} r^{-2} dr - \int_{b}^{\infty} \left[ 1 - \frac{b^{2}}{r^{2}} \right]^{-1/2} r^{-2} dr \]

If \( b > n\rho, \) so \( r_c = b/n > \rho, \) this is identical with the square well case; if \( b < n\rho, \) so \( r_c = \rho, \) we have
\[ \chi = -2b \left\{ \begin{array}{l} \int_0^\sigma \left[ \frac{2}{n^2} - \frac{b^2}{r^2} \right]^{-1/2} r^{-2} dr \\ \int_0^\sigma \left[ 1 - \frac{b^2}{r^2} \right]^{-1/2} r^{-2} dr \end{array} \right\} \]

The second and third terms are those for the square well case, and the first one is

\[ \frac{2b}{n} \left\{ \int_0^{\sigma} \left[ \frac{2}{n^2} - \frac{b^2}{r^2} \right]^{-1/2} r^{-1} dr \right\} = 2 \arccos \left( \frac{b}{n} \right). \]

as expected. In Fig. 18-5, the introduction of the repulsive core merely produces additional "edge scattering".

For the step barrier potential, as long as \( E < \varepsilon \) the deflection is identical to that for the hard sphere case. When the incident energy is above the step, \( E > \varepsilon \), however, we may define an index of refraction

\[ n = \left( 1 - \frac{\varepsilon}{E} \right)^{1/2} \]

such that \( 0 < n < 1 \). The turning point is then given by \( r_c = b/n \) and the deflection angle has the same form as for the square well case.

\[ \chi = -2 \arccos \left( \frac{b}{n\sigma} \right) + 2 \arccos \left( \frac{b}{\sigma} \right). \]

Now, however, since \( n < 1 \), the second term dominates, so that \( \chi \) is always positive. The differential cross section for \( E > \varepsilon \) has the same form as that for the square well case, as given in (18-16). Furthermore, we find that if

\[ \frac{n}{\text{step barrier}} = \frac{1}{n \text{ square well}} \]

then the angular distributions are identical except for a scale factor, that is
$$u(x^2/n^2)_{\text{step barrier}} = (u(x)/n^2)_{\text{square well}}$$

Finally, we may consider the "stairstep potential" illustrated in Fig. 18-7.

For this we readily find that when

$$n_{j+1} \sigma_{j+1} < b < n_j \sigma_j,$$

that is, when

$$\sigma_{j+1} < r_c < \sigma_j,$$

then

$$\chi = \sum_{i=0}^{j} \left[ \frac{\pi}{2} \arccos \frac{b}{n_i - \sigma_i} + \frac{2 \pi}{n_i} \arccos \frac{b}{n_i \sigma_i} \right]$$

where the sum extends from $i = 0$ to $i = j$. This potential corresponds to a "painted sphere" coated with layers with various indices of refraction.

Since an arbitrary potential can be approximated fairly well by choosing a sufficiently large number of stairsteps, this formula might be quite useful for computer calculations.