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A Specific Example: Scattering from Spherical Square Well Potentials

To solve a very specific example, let us look first at the scattering from a spherical square well potential, with

$$V(r) = V_0 \quad \text{for } r \leq a, \qquad V(r) = 0 \quad \text{for } r > a, \tag{1}$$

(see Fig. 43.1), where the constant V_0 could be either negative (attractive potential) or positive (repulsive potential), including $V_0 = +\infty$, the so-called hard sphere case. The latter might be a good approximation for the scattering of noble gas atoms from noble gas atoms. In this case, classical scattering theory would be sufficient for gases at temperatures such that $\lambda \ll a$. Quantum theory would be needed only for $\lambda \simeq a$ or $\lambda > a$. For noble gas atoms with mass, m, at an absolute temperature, T,

$$\begin{aligned}\frac{\lambda}{2\pi} = \frac{\hbar}{p} \simeq \frac{\hbar}{[mkT]^{\frac{1}{2}}} = \frac{\hbar c}{[mc^2kT]^{\frac{1}{2}}} &= \frac{1.97\times 10^3 eV \times 10^{-8} cm}{[M(.94\times 10^9 eV)\times \frac{1}{40} eV \frac{T}{300}]^{\frac{1}{2}}}\\ &\approx \frac{7\times 10^{-8} cm}{\sqrt{MT}},\end{aligned} \tag{2}$$

where M is the mass number of the atom in atomic units. Thus, quantum theory is needed only for the lightest atoms, e.g., He with $M = 4$, at extremely low temperatures.

For the general $V(r)$, the asymptotic form of the solution, as $r \to \infty$, is

$$\begin{aligned}R_l(kr) = \frac{w_l(kr)}{kr} &\to i^l e^{i\delta_l}(2l+1)\frac{\sin(kr - \frac{\pi}{2}l + \delta_l)}{kr}\\ &= i^l e^{i\delta_l}(2l+1)\big(j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l\big),\end{aligned} \tag{3}$$

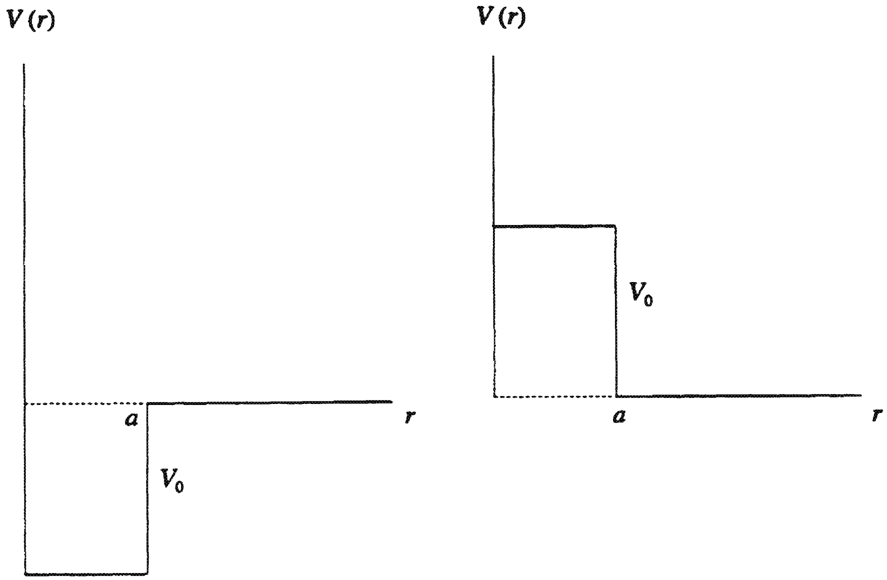

FIGURE 43.1. Square well potential scatterers.

where we have used the asymptotic forms for j_l and n_l, eq. (44) of Chapter 41. Now for the square well problem, the solution for $R_l(kr)$ is a linear combination of the free-wave radial functions, $j_l(kr)$ and $n_l(kr)$, for *all* values of $r \geq a$, so our solution for $r \geq a$ is

$$R_l(kr) = i^l e^{i\delta_l}(2l+1)\big(j_l(kr)\cos\delta_l - n_l(kr)\sin\delta_l\big). \tag{4}$$

We shall also need, again in the region $r \geq a$,

$$\left(r\frac{dR_l}{dr}\right) = (kr)i^l e^{i\delta_l}(2l+1)\big(j_l'(kr)\cos\delta_l - n_l'(kr)\sin\delta_l\big). \tag{5}$$

All of the information from the interior region will be related to the ratio, evaluated at the boundary $r = a$, of the quantity

$$\begin{aligned}\left[\frac{1}{R_l}r\frac{dR_l}{dr}\right]_{r=a} \equiv \beta_l &= (ka)\left[\frac{(j_l'\cos\delta_l - n_l'\sin\delta_l)}{(j_l\cos\delta_l - n_l\sin\delta_l)}\right]_{r=a}\\ &= (ka)\left[\frac{(j_l'+in_l')e^{2i\delta_l} + (j_l'-in_l')}{(j_l+in_l)e^{2i\delta_l} + (j_l-in_l)}\right]_{r=a}.\end{aligned} \tag{6}$$

Solving this for the phase shift,

$$e^{2i\delta_l} = -\left[\frac{(j_l - in_l)}{(j_l+in_l)}\left[\frac{1-\frac{ka}{\beta_l}\left(\frac{j_l'-in_l'}{j_l-in_l}\right)}{1-\frac{ka}{\beta_l}\left(\frac{j_l'+in_l'}{j_l+in_l}\right)}\right]\right]_{r=a}. \tag{7}$$

A Hard Sphere Scattering

For the hard sphere case, we must have $R_l(ka) = 0$, and $\frac{dR_l}{dr}$ must be finite at $r = a$. Thus, $\beta_l = \infty$, and

$$e^{2i\delta_l^{\text{H.Sph}}} = -\left[\frac{(j_l(ka) - in_l(ka))}{(j_l(ka) + in_l(ka))}\right] = \left[\frac{(n_l(ka) + ij_l(ka))}{(n_l(ka) - ij_l(ka))}\right] = \frac{e^{i\delta_l^{\text{H Sph.}}}}{e^{-i\delta_l^{\text{H Sph.}}}}, \tag{8}$$

so

$$\tan\delta_l^{\text{H.Sph.}} = \frac{j_l(ka)}{n_l(ka)}. \tag{9}$$

For the low-energy limit [see eq. (45) of Chapter 41],

$$\tan\delta_l^{\text{H.Sph.}} = \frac{\frac{2^l l!}{(2l+1)!}(ka)^l\left(1 - \frac{(ka)^2}{2(2l+3)} + \cdots\right)}{-\frac{(2l)!}{(ka)^{l+1}2^l l!}\left(1 + \frac{(ka)^2}{2(2l-1)} + \cdots\right)}. \tag{10}$$

Again, in the low-energy limit δ_0 dominates. Note that $\tan\delta_0^{\text{H.Sph.}} = -\tan(ka)$; and for all (ka)

$$\delta_0^{\text{H.Sph.}} = -(ka), \tag{11}$$

whereas, for $(ka) \ll 1$,

$$\delta_1^{\text{H.Sph.}} \simeq -\frac{(ka)^3}{3} + \cdots. \tag{12}$$

In the extreme low-energy limit, neglecting all but the $l = 0$ phase shift,

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2\delta_0}{k^2} = a^2, \qquad \sigma = 4\pi a^2. \tag{13}$$

In next approximation, with $(ka) \ll 1$,

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\left(\sin^2\delta_0 + 3\delta_1\sin 2\delta_0\cos\theta + \cdots\right) = a^2\left(\left[1 - \frac{(ka)^2}{3}\right] + 2(ka)^2\cos\theta\right). \tag{14}$$

As (ka) increases, the differential cross section will show more and more angular oscillations, as more and more terms in the l sum contribute. Fig. 43.2 shows the θ dependence of the differential cross section for a very large value of (ka), as well as the limit of extremely large (ka). In this extreme short-wavelength limit, the differential cross section has the classical value, $\frac{a^2}{4}$, for all values of $\theta > \theta_{\text{min.}} \approx (\pi/(ka))$. The total cross section is

$$\sigma_{ka\to\infty} = 2\pi a^2, \tag{15}$$

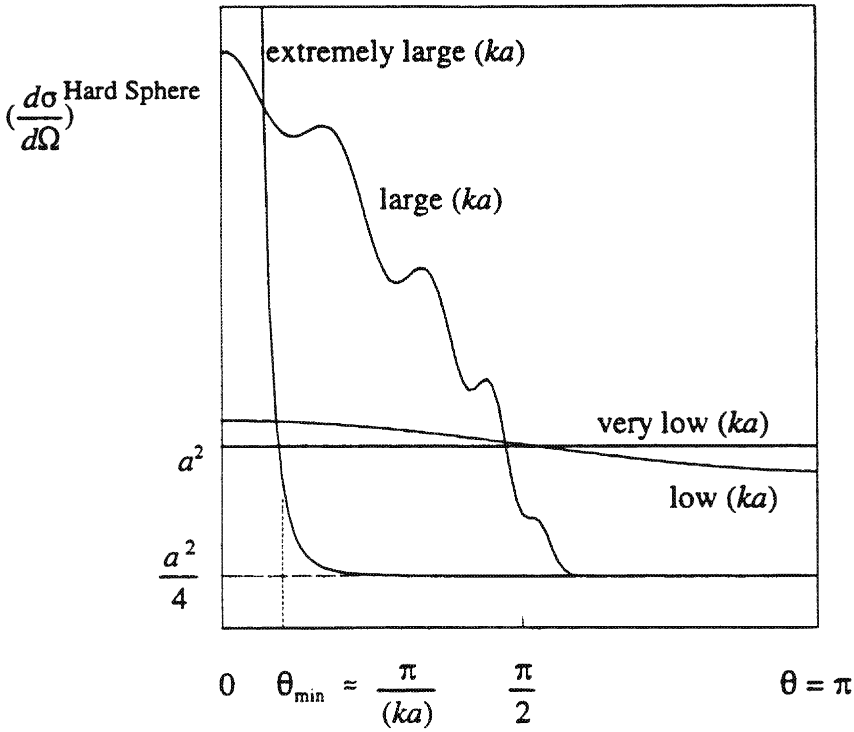

FIGURE 43.2. Hard sphere differential scattering cross sections.

that is, twice the classical value: one unit of πa^2 coming from the forward peak for $\theta < \theta_{\text{min.}}$; the second unit of πa^2 coming from all values of θ from the constant value of $\frac{a^2}{4}$ for $\frac{d\sigma}{d\Omega}$. The strong forward peak giving the extra factor of πa^2 comes from the wave description of even the classical limit. Our wave function now consists of essentially three components, a plane wave extending through *all* of space, a "true" scattered wave showing an isotropic scattering with equal probability in all directions, and a strongly forward-peaked wave interfering with the plane wave in the forward direction to make the geometrical shadow. (See Fig. 43.3.)

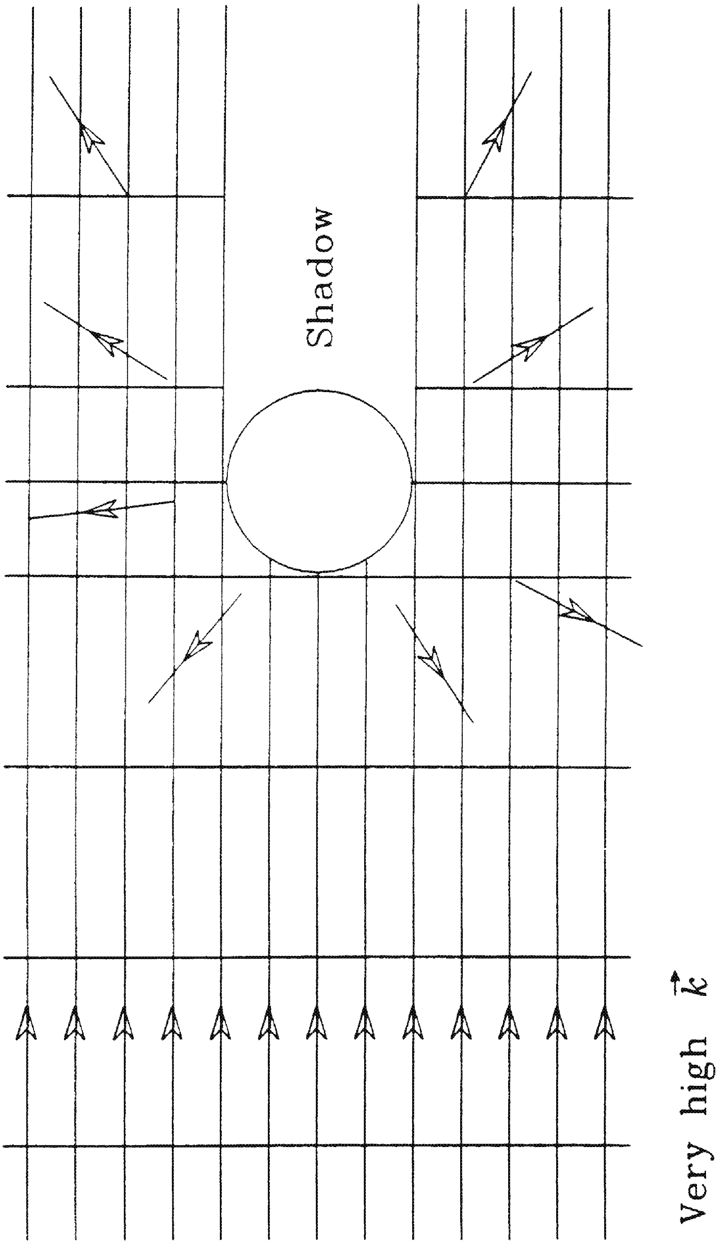

FIGURE 43.3. Hard sphere scattering, high k limit.

B The General Case: Arbitrary V_0

In the general case, we can express the phase shifts, δ_l, by

$$e^{2i\delta_l} = e^{2i\delta_l^{\text{H.Sph.}}} \frac{\beta_l - (ka)\left(\frac{j_l' - in_l'}{j_l - in_l}\right)_{r=a}}{\beta_l - (ka)\left(\frac{j_l' + in_l'}{j_l + in_l}\right)_{r=a}}, \tag{16}$$

that is, δ_l is determined exclusively from the quantity β_l. From the continuity of the wave function and its first derivative at $r = a$, we get

$$\beta_l = (k_0 a)\frac{j_l'(k_0 a)}{j_l(k_0 a)}, \qquad \text{with} \quad k_0^2 = \frac{2\mu(E - V_0)}{\hbar^2}, \tag{17}$$

where we have also used the fact that the interior solution, for $r < a$, must be regular at the origin. Using the abbreviation for the quantity

$$(ka)\left(\frac{j_l' + in_l'}{j_l + in_l}\right)_{r=a} \equiv (\Delta_l + is_l), \tag{18}$$

we have

$$e^{2i\delta_l} = e^{2i\delta_l^{\text{H.Sph.}}} \frac{\beta_l - \Delta_l + is_l}{\beta_l - \Delta_l - is_l} = e^{2i\delta_l^{\text{H.Sph.}}}\left(1 + \frac{2is_l}{\beta_l - \Delta_l - is_l}\right). \tag{19}$$

The quantities Δ_l, s_l, and $e^{i\delta_l^{\text{H.Sph.}}}$ are all known functions of ka and completely independent of the strength of the potential. Moreover, they are all smooth functions of ka. For example, for $l = 0$,

$$\delta_0^{\text{H.Sph.}} = -ka, \qquad \Delta_0 = -1, \qquad s_0 = ka. \tag{20}$$

For $l = 1$,

$$e^{i\delta_1^{\text{H.Sph.}}} = e^{-ika}\frac{(1 + ika)}{[1 + (ka)^2]^{\frac{1}{2}}}, \quad \Delta_1 = -\frac{[2 + (ka)^2]}{[1 + (ka)^2]}, \quad s_1 = \frac{(ka)^3}{[1 + (ka)^2]}. \tag{21}$$

To express the differential and total cross sections as functions of $\delta_l^{\text{H.Sph.}}$, Δ_l, s_l, and β_l, it will be useful to use the identity

$$e^{i\delta_l}\sin\delta_l = \frac{i}{2}(1 - e^{2i\delta_l}) \tag{22}$$

to rewrite

$$e^{i\delta_l}\sin\delta_l = e^{i\delta_l^{\text{H.Sph}}}\sin\delta_l^{\text{H.Sph.}} + \frac{s_l e^{2i\delta_l^{\text{H.Sph.}}}}{\beta_l - \Delta_l - is_l}. \tag{23}$$

This equation leads to an expression for the l^{th} partial cross section

$$\sigma_l = \frac{4\pi}{k^2}(2l + 1)\left(\sin^2\delta_l^{\text{H.Sph.}} + \frac{s_l^2(1 - 2\sin^2\delta_l^{\text{H.Sph.}})}{(\beta_l - \Delta_l)^2 + s_l^2} + \frac{s_l(\beta_l - \Delta_l)\sin 2\delta_l^{\text{H.Sph.}}}{(\beta_l - \Delta_l)^2 + s_l^2}\right). \tag{24}$$

Because Δ_l, s_l, and $\delta_l^{\text{H.Sph.}}$, especially for low values of l, are mild functions of (ka), any rapid changes in $\delta_l(k)$ with k, and hence σ_l with k, must be caused by a strong k dependence in β_l. In particular, β_l can go to infinity for particular values of k for which $R_l(ka) = 0$. This process leads us to the next topic.