S-Wave Scattering off a Square-Well Potential

The potential is

$$V(r) = -V_0 \qquad \text{for } r < r_0$$
$$V(r) = 0 \qquad \text{for } r > r_0$$

where $V_0 > 0$. Let

$$k_0 = \sqrt{\frac{2\mu V_0}{\hbar^2}} \quad \text{so that} \quad V_0 = \frac{\hbar^2 k_0^2}{2m}.$$

The wave function $\psi(x) = R(r) = u_{k,0}(r)/r$ must satisfy for positive energy $E = \frac{(\hbar k)^2}{2m}$

$$\left[-\frac{\hbar^2}{2m}\Delta - V_0\right]\frac{u_{k,0}(r)}{r} = \frac{\hbar^2 k^2}{2m}\frac{u_{k,0}(r)}{r} \qquad r < r_0$$

Now

$$\Delta \frac{u}{r} = \frac{1}{r} u'', \quad \text{so we have}$$

$$-\frac{\hbar^2}{2m} u''_{k,0}(r) - V_0 u_{k,0}(r) = \frac{\hbar^2 k^2}{2m} u_{k,0}(r)$$

$$-u'' - \frac{2m}{\hbar^2}\frac{\hbar^2 k_0^2}{2m} u = k^2 u \qquad \text{or}$$

$$u'' + (k_0^2 + k^2)\, u = 0 \qquad \text{for } r < r_0$$

and

$$u'' + k^2 u = 0 \qquad \text{for } r > r_0$$

Since $u_{k,0}(0)=0$, the solution for $r<r_0$ is

$$u(r) = B\sin k'r \qquad k'=\sqrt{k_0^2+k^2}.$$

For $r>r_0$

$$u(r) = A\sin(kr+\delta_0).$$

We require that the logarithmic derivatives match

$$\frac{(B\sin k'r)'}{B\sin k'r} = \frac{[A\sin(kr+\delta_0)]'}{A\sin(kr+\delta_0)} \quad \text{at } r_0$$

so

$$k'\cot k'r_0 = k\cot(kr_0+\delta_0) \equiv k\cot\alpha(k).$$

Then

$$\frac{1}{k'}\tan k'r_0 = \frac{1}{k}\tan\alpha(k) \qquad (\delta_0)$$

or

$$\alpha(k) = \tan^{-1}\left[\frac{k}{k'}\tan(k'r_0)\right]$$

or

$$\delta_0(k) = \tan^{-1}\left[\frac{k}{k'}\tan k'r_0\right] - kr_0. \qquad (\delta_1)$$

This is the s-wave phase shift, and the s-wave x-section is

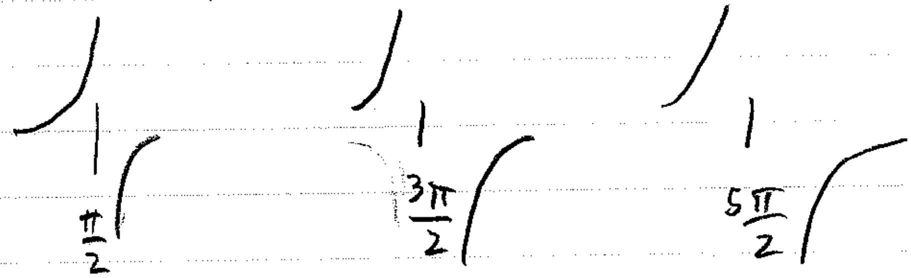
$$\sigma_0(k) = \frac{4\pi}{k^2}\sin^2\delta_0(k).$$

At very low energies, $k \simeq 0$ and

$$k' = \sqrt{k_0^2 + k^2} \simeq k_0 .$$

So when $k r_0 = (2n+1)\frac{\pi}{2}$

$$\tan k' r_0 \simeq \tan k r_0 = \tan (2n+1)\frac{\pi}{2}$$



and so

$$\delta_0(k) = \tan^{-1}\left[\frac{k}{k'} \tan k' r_0\right] - k r_0 \simeq (2n+1)\frac{\pi}{2}$$

and the s-wave x-section

$$\sigma_0(k) = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_0(k)$$

$$= \frac{4\pi}{k^2}(2l+1)\sin^2(2n+1)\frac{\pi}{2}$$

$$= \frac{4\pi}{k^2}(2l+1)$$

is maximal when $r_0 k' \simeq r_0 k_0 \simeq (2n+1)\frac{\pi}{2}$.

Poles in $S_0(k) = e^{2i\delta_0(k)}$

Note that

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

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

So
$$e^{2i(kr_0+\delta_0)} = \frac{\cot(kr_0+\delta_0)+1}{\cot(kr_0+\delta_0)-i}$$

$$= \frac{\frac{k'}{k}\cot k'r_0 + 1}{\frac{k'}{k}\cot k'r_0 - i}.$$

So the s-wave S-matrix element is

$$S_0(k) = e^{2i\delta_0} = e^{-2ikr_0}\left(\frac{\cos k'r_0 + \frac{k}{k'}\sin k'r_0}{\cos k'r_0 - i\frac{k}{k'}\sin k'r_0}\right) \qquad (\delta_2)$$

which has poles in complex k when $\cos k'r_0 - ik\sin k'r_0/k' = 0.$ $\qquad (P_1)$

The Bound States

Let $\quad k = i k'' \qquad E = \dfrac{\hbar^2 k^2}{2\mu} = -\dfrac{\hbar^2 k''^2}{2\mu} < 0.$

For $r < r_0$

$$u(r) = D \sin k' r$$

$$k'^2 = k_0^2 + k^2 = k_0^2 - k''^2$$

For $r > r_0$

$$u(r) = C e^{-k'' r}.$$

Continuity of the logarithmic derivatives gives

$$\frac{-k'' C e^{-k'' r}}{C e^{-k'' r}} = k' \frac{D \cos k' r}{D \sin k' r} \qquad \text{at } r = r_0$$

so

$$-k'' = k' \cot k' r_0 \qquad (P_2)$$

or

$$k' \cos k' r_0 + k'' \sin k' r_0 = 0$$

or since $k'' = -ik$

$$k' \cos k' r_0 - ik \sin k' r_0 = 0$$

which is the equation (P_1) for the poles in the s-wave S-matrix element $S_0(k)$.
So $S_0(k)$ has poles at the s-wave bound states, $k = ik''$.

This result is part of a pattern:

For potentials $V(r)$ that fall off with r as $r \to \infty$ sufficiently fast, the poles of the lth-wave S-matrix $S_l(k)$ are at the bound states of the lth partial wave

$$E = \frac{\hbar^2 k^2}{2m} < 0 \qquad k = ik'', \quad k'' > 0.$$

The Scattering Length

The scattering length a is defined as the low-energy limit of the s-wave phase shift $\delta_0(k)$ divided by k

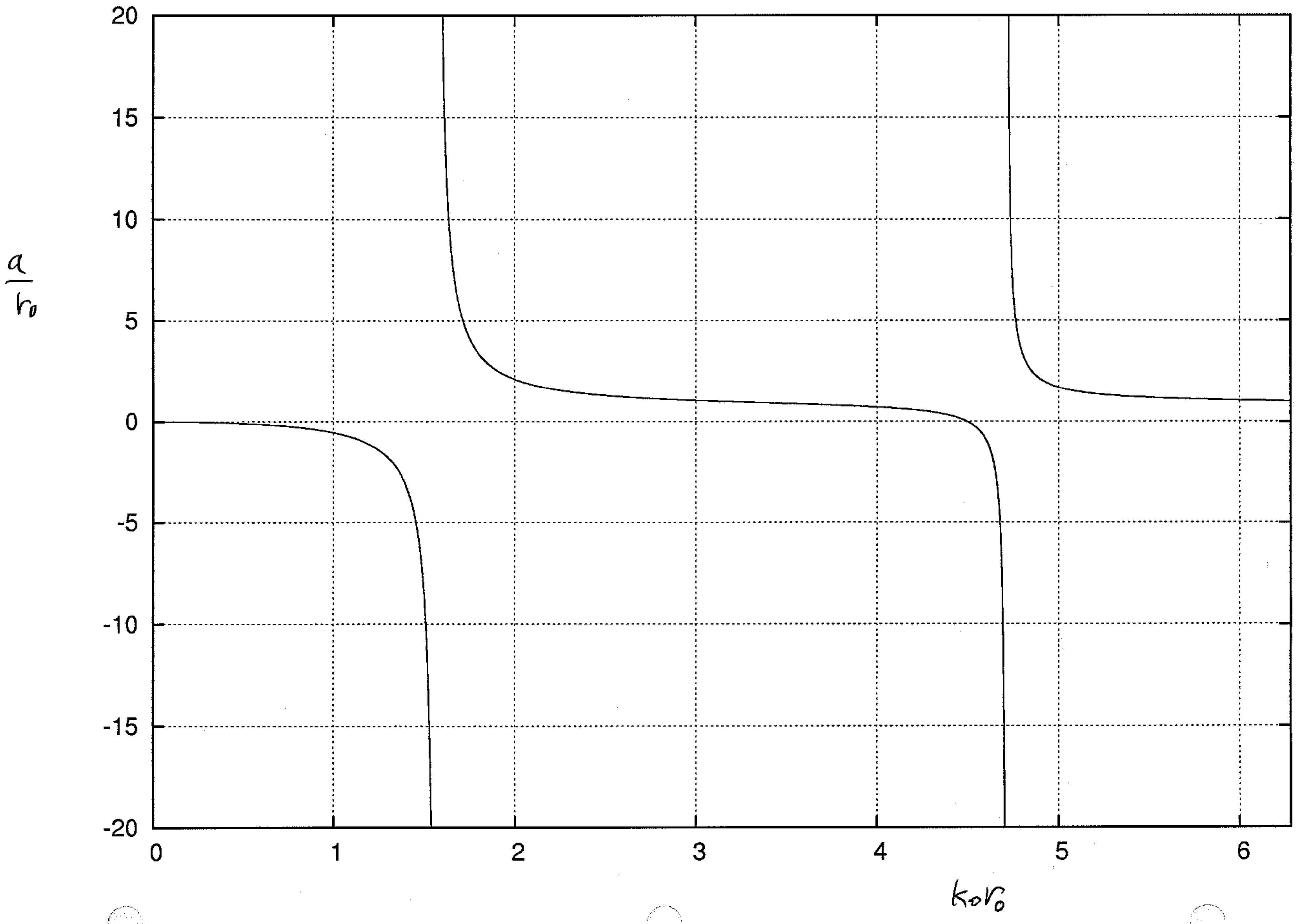
$$a \equiv - \lim_{k \to 0} \frac{\delta_0(k)}{k} .$$

We let $k \to 0$ in Eq (δ_0)

$$\frac{\tan \sqrt{k^2 + k_0^2}\, r_0}{\sqrt{k^2 + k_0^2}} = \frac{\tan\left(k r_0 + \delta_0(k)\right)}{k}$$

$$k r_0 + \delta_0(k) = \frac{k}{k_0} \tan k_0 r_0$$

$$\delta_0(k) = -k r_0 + \frac{k}{k_0} \tan k_0 r_0$$



$\frac{a}{r_0}$
20
15
10
5
0
-5
-10
-15
-20
0
1
2
3
4
5
6
$k_0 r_0$

or

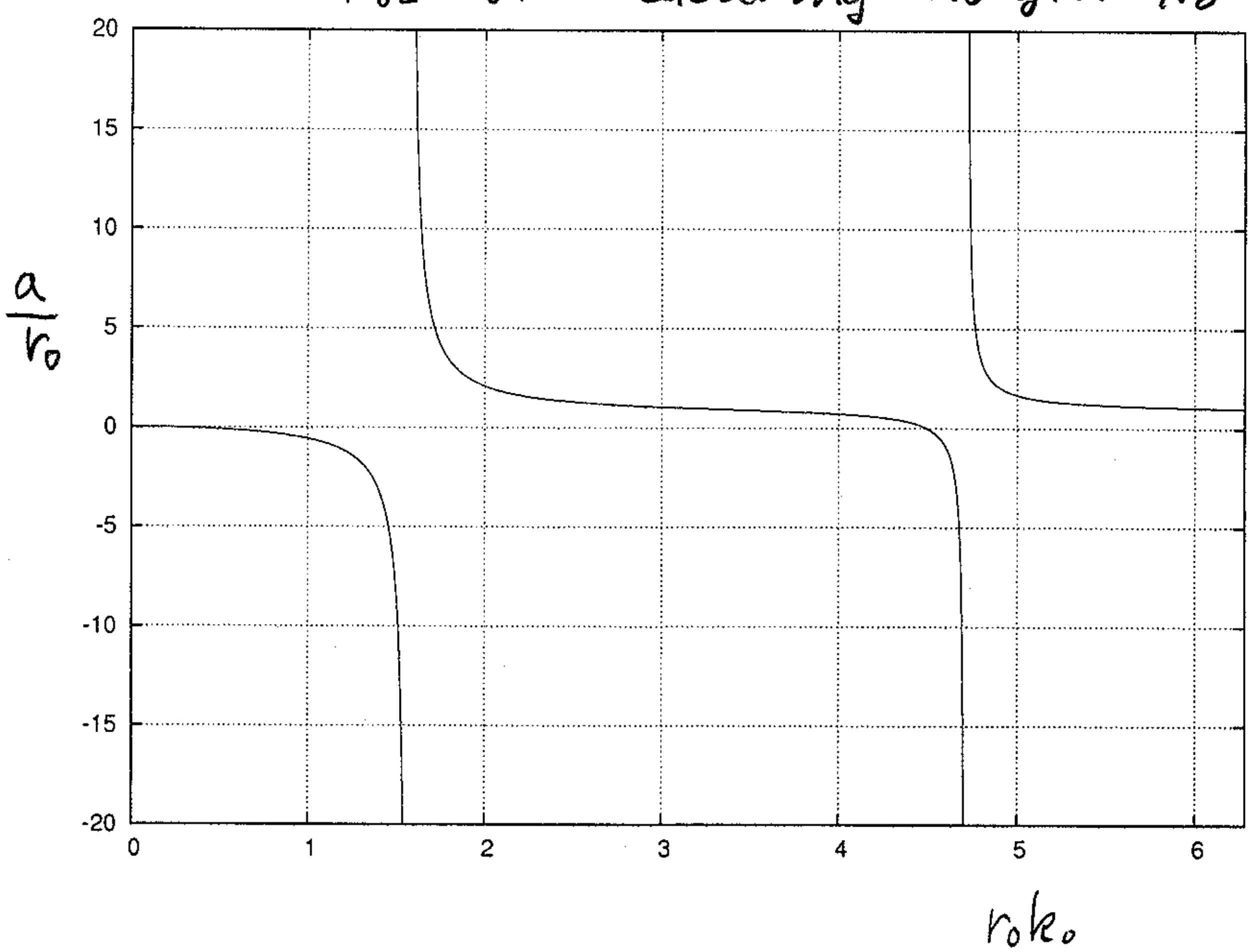
$$\delta_0(k) = -k\left(r_0 - \frac{\tan k_0 r_0}{k_0}\right)$$

So the scattering length is

$$a = r_0\left(1 - \frac{\tan k_0 r_0}{k_0 r_0}\right).$$

Here's what $\frac{a(k_0 r_0)}{r_0}$ looks like this:

Plot of Scattering Length a/r_0



The scattering length a has poles when

$$k_0 r_0 = (2n+1)\frac{\pi}{2}$$

since

$$\tan(2n+1)\frac{\pi}{2} = \pm\infty .$$

Recall that the bound-state condition (P_2) was

$$-k'' = k' \cot k' r_0$$

or

$$\tan r_0\sqrt{k_0^2 - k''^2} = -\frac{\sqrt{k_0^2 - k''^2}}{k''}$$

$$= -\sqrt{\frac{k_0^2}{k''^2} - 1}$$

in which $0 \le k'' \le k_0$ and $E = -\frac{\hbar^2 k''^2}{2m} < 0.$

This condition is

$$\frac{\tan r_0\sqrt{k_0^2 - k''^2}}{r_0\sqrt{k_0^2 - k''^2}} = -\frac{1}{r_0 k''}.$$

Now as we increase k_0, the first bound state will appear as a barely bound state with $k'' \approx 0$. That happens when

$$\frac{\tan r_0 k_0}{r_0 k_0} \approx \infty \quad \text{and so} \quad r_0 k_0 = \frac{\pi}{2}.$$

Similarly, the second bound state will appear when k_0 has been raised enough, and it will appear with $k'' \approx 0$ when

$$r_0 k_0 = \frac{3\pi}{2}.$$

So as we deepen the depth V_0 of the potential well, new bound states appear when

$$r_0 k_0 = (2n+1)\frac{\pi}{2}$$

and at each one, the scattering length

$$a = -\lim_{k \to 0} \frac{\delta_0(k)}{k} \quad \text{diverges.}$$

And for low k, the s-wave x-section

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

is maximal because $\delta_0(k) \approx (2n+1)\pi/2$.