8.322: Quantum Theory II

Problem Set #10 Solutions
May 8, 2007

1. **The density of states and the phase shift**

(a) For $r > b$, the potential is zero. Hence the radial wavefunction is

$$R_l(r) = a_l j_l(kr) + b_l n_l(kr) \xrightarrow{r\to\infty} c_l \cdot \frac{\sin(kr - \frac{l\pi}{2} + \delta_l(k))}{kr}$$

Since the particle is confined in the sphere of radius R, we have $R_l(R) = 0$.

$$\sin\left(k_n R - \frac{l\pi}{2} + \delta_l(k_n)\right) = 0$$

from which we immediately obtain

$$k_n R + \delta_l(k_n) = \left(n + \frac{l}{2}\right)\pi$$

(b) For $V \equiv 0$, the phase shifts are zero. If R is large, the energy levels are sufficiently dense. Thus,

$$\Delta E \approx \frac{dE}{dn} = \frac{d}{dn}\left(\frac{\hbar^2 k^2}{2m}\right) = \frac{\hbar^2 k}{m} \cdot \frac{dk}{dn}$$

From (a),

$$k_n R + \delta_l(k_n) = \left(n + \frac{l}{2}\right)\pi$$

$$\frac{dk}{dn}R + \frac{d\delta_l(k)}{dk} \cdot \frac{dk}{dn} = \pi$$

and thus

$$\frac{dk}{dn} = \frac{\pi}{R + \frac{d\delta_l(k)}{dk}}$$

Hence,

$$\Delta E \approx \frac{\hbar^2 k}{m} \frac{\pi}{R + \frac{d\delta_l(k)}{dk}}$$

Therefore,

$$\Delta E - \Delta E_0 \approx \frac{\hbar^2 k\pi}{m}\left(\frac{1}{R + \frac{d\delta_l(k)}{dk}} - \frac{1}{R}\right) \approx \frac{\hbar^2 k\pi}{m}\left(-\frac{1}{R^2}\frac{d\delta_l(k)}{dk}\right)$$

setting $\hbar = 1$,

$$\Delta E - \Delta E_0 \approx -\frac{k\pi}{mR^2}\frac{d\delta_l(k)}{dk}$$

(c) For a given l angular momentum there are $2l+1$ degenerate states. Hence,

$$\frac{d\Delta n_l}{dk} = \frac{dn_l}{dk} - \frac{dn_{l0}}{dk} = \left[\frac{1}{\pi}\left(R + \frac{d\delta_l(k)}{dk}\right) - \frac{R}{\pi}\right](2l+1) = \frac{2l+1}{\pi}\cdot\frac{d\delta_l(k)}{dk}$$

(d) We know that

$$S = \mathrm{diag}(e^{2i\delta_l(k)})$$

Thus,

$$\mathrm{Tr}(\ln S) = \sum_l (2l+1)\ln(e^{2i\delta_l(k)}) = \sum_l (2l+1)2i\delta_l(k)$$

$$\frac{1}{2\pi i}\frac{d}{dk}\mathrm{Tr}(\ln S) = \sum_l \frac{2l+1}{\pi}\frac{d\delta_l(k)}{dk}$$

On the other hand,

$$\frac{d\Delta n_l}{dk} = \frac{2l+1}{\pi}\cdot\frac{d\delta_l(k)}{dk}$$

Thus we obtain

$$\frac{d\Delta n_l}{dk} = \frac{1}{2\pi i}\frac{d}{dk}\mathrm{Tr}(\ln S)$$

where $n(k)$ is the total density of states.

2. **Levinson's Theorem — an example**

(a) Recall that

$$\frac{d\Delta n_l}{dk} = \frac{2l+1}{\pi}\cdot\frac{d\delta_l(k)}{dk}$$

Integrating from $k=0$ to $k=\infty$ gives the total change in the number of scattering states

$$\Delta n_l = \frac{2l+1}{\pi}(\delta_l(\infty) - \delta_l(0))$$

Hence by Levinson's theorem,

$$\Delta n_l + N_l(\mathrm{bound}) = 0$$

Without a potential, there are no bound states. Thus, the above equation tells us that the total number of states with angular momentum l remains invariant when a potential is introduced.

(b) For the attractive potential hole, we have inside the region $r < b$

$$R(r) = j_0(qr) = \frac{\sin(qr)}{qr}$$

where $q = \sqrt{k^2 + 2mV_0/\hbar^2}$. Outside ($r > b$) we have

$$R(r) = Aj_0(kr) + Bn_0(kr) = \frac{C}{kr}\sin(kr + \delta_0(k))$$

Matching

$$R(b-0) = R(b+0)$$
$$R'(b-0) = R'(b+0)$$

gives

$$\frac{C}{kb}\sin(kb + \delta_0(k)) = \frac{\sin(qb)}{qb}$$
$$\frac{C}{b}\cos(kb + \delta_0(k)) = \frac{1}{b}\cos(qb)$$

Taking their quotient,

$$\frac{1}{k}\tan(kb + \delta_0(k)) = \frac{1}{q}\tan(qb)$$

which is the desired result.

(c) When $k \to \infty$, $q \approx k$ so we have

$$\frac{1}{k}\tan(kb + \delta_0(k)) = \frac{1}{k}\tan(kb)$$

Hence,

$$\lim_{k\to\infty}\delta_0(k) = n\pi \qquad n \in \mathbb{Z}$$

At first sight there is an ambiguity. But since

$$\lim_{U\to 0}\delta_0(k) = 0$$

and because the limit $k \to \infty$ is equivalent to $U \to 0$, we must have

$$\lim_{k\to\infty}\delta_0(k) = 0.$$

In other words, for $k^2 \gg U$

$$\delta_0(kb) = \arctan\left((1 - \frac{U}{2k^2})\tan(kb + \frac{Ub}{2k})\right) - kb$$

At $U = 0$, this gives zero and thus fixes the branch of the arcus tangent function. So

$$\delta_0(kb) = 0 + \mathcal{O}(U/k^2) \xrightarrow{k\to\infty} 0$$

(d) The bound state has wave functions

$$rR_0(r) = A\sin(qr) \qquad \text{for } r < b$$

$$rR_0(r) = Be^{-\kappa r} \qquad \text{for } r > b$$

where $q = \frac{1}{\hbar}\sqrt{2m(V_0 - E)}$ and $\kappa = \frac{1}{\hbar}\sqrt{2mE}$. When a new bound state appears, its energy is close to zero (weakly bound). Thus,

$$\kappa = 0$$

and from the matching of wavefunctions

$$\sin(qb) = \pm 1$$

and hence

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

from which the values of U at which new bound states appear are

$$U_n = \frac{(2n+1)^2\pi^2}{4b^2}$$

(e) Near $k = 0$, $q \approx \sqrt{U}$ and we have

$$\tan(kb + \delta_0(k)) = \frac{k}{\sqrt{U}}\tan(b\sqrt{U})$$

Introducing $z = kb$,

$$\frac{\tan(z + \delta_0(z))}{z} = \frac{\tan(b\sqrt{U})}{b\sqrt{U}} \tag{0.1}$$

Taylor–expansion of the phase shift gives

$$\delta_0(z) \approx n\pi + az$$

with $a \neq 0$ in the general case, since otherwise the LHS of (0.1) equals to one (by L'Hôpital's rule). The different slopes are parameterized by the value of $b\sqrt{U}$

$$a = a(b\sqrt{U})$$

Now fix z to a small but finite value and change U. As $b\sqrt{U}$ crosses $(n + \frac{1}{2})\pi$, the RHS of (0.1) changes from large positive value to large negative value. Since $\delta_0(k)$ is continuous in U, it should jump from the branch

$$\left(n\pi - \frac{\pi}{2},\ \ n\pi + \frac{\pi}{2}\right)$$

to

$$\left((n+1)\pi - \frac{\pi}{2},\ \ (n+1)\pi + \frac{\pi}{2}\right)$$

The phase shift is plotted in Figure 1 as a function of k.

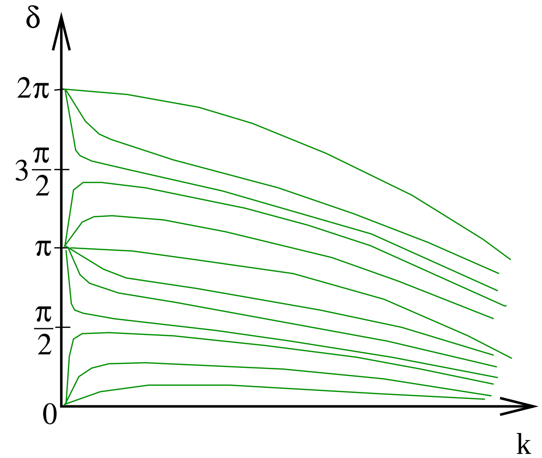

Figure 1: The phase shift as a function of k.

3. **WKB approximation phase shifts**

(a) For the s–wave,

$$\Psi = Y_{00}(\theta, \phi) R(r)$$

Let

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

Then u satisfies a Schrödinger–like equation

$$-\frac{\hbar^2}{2m} u'' + V(r) u = \frac{\hbar^2 k^2}{2m} u$$

for which we can apply WKB. Hence,

$$u(r) = \frac{c_+}{\sqrt{p(r)}} \exp\left(\frac{i}{\hbar} \int p(\xi) d\xi\right) + \frac{c_-}{\sqrt{p(r)}} \exp\left(-\frac{i}{\hbar} \int p(\xi) d\xi\right)$$

where $p(r) = \sqrt{2m(E - V(r))}$. From boundary conditions, $c_\pm = \pm\frac{1}{2i}$ and thus

$$u(r) = \frac{1}{\sqrt{p(r)}} \sin\left(\frac{1}{\hbar} \int p(\xi) d\xi\right)$$

Substituting p gives

$$\int_0^r p(\xi) d\xi = \int_0^r \sqrt{2m(E - V(\xi))} d\xi = \hbar k \left[\int_0^r \left(\sqrt{1 - \frac{V(\xi)}{E}} - 1\right) d\xi + r\right]$$

Therefore

$$u(r) = \frac{1}{\sqrt{p(r)}} \sin\left(kr + k \int_0^r \left(\sqrt{1 - \frac{2mV(\xi)}{\hbar^2 k^2}} - 1\right) d\xi\right)$$

from which we see that

$$\delta_0(k) = k\int_0^\infty \left(\sqrt{1-\frac{2mV(\xi)}{\hbar^2k^2}}-1\right)d\xi$$

For $k=0$,

$$\delta_0(k) = \frac{1}{\hbar}\int_0^\infty \sqrt{2m|V(\xi)|}d\xi$$

For $k\to\infty$,

$$\delta_0(k) = k\int_0^\infty \frac{mV(\xi)}{\hbar^2 k}d\xi \to 0$$

Thus by Levinson's theorem,

$$N_0(\text{bound}) \approx \frac{1}{\hbar\pi}\int_0^\infty \sqrt{2m|V(r)|}dr = \frac{1}{\pi}\int_0^\infty \sqrt{U(r)}dr$$

which agrees with the sum rule derived in PS#5.

(b) The function $u(r)$ satisfies a Schrödinger equation with potential $V(r)$ and boundary condition $u(0)=0$ which is identical to that of problem 1 of PS#5. Thus the phase shifts are the same.

(c) As $k\to\infty$, the effect of the potential on the wavefunction becomes negligible. Hence,

$$\delta_0(\infty)\approx 0$$

By Levinson's theorem,

$$\delta_0(0)-\delta_0(\infty) = \pi N_0(\text{bound}) = 0$$

since there are no bound states. This immediately gives

$$\delta_0(0)=\delta_0(\infty)=0$$

(d) The potential, with the three special values of the energy, is shown in Figure 2.

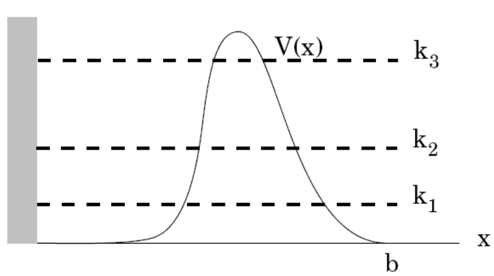

Figure 2: The potential.

For **small** k (below the top of the barrier), we can apply the results of problem 1 of PS#5

$$\delta_0(k) = 2\pi n + \frac{1}{\hbar}\int_{x_0}^{\infty}\left(\sqrt{\hbar^2k^2 - 2mV(\xi)} - \hbar k\right)d\xi - kx_0 + \frac{\pi}{4}$$

where x_0 is the classical turning point s.t. $V(x_0) = \frac{\hbar^2k^2}{2m}$.

$$\delta_0(k) = 2\pi n + \frac{1}{\hbar}\int_{x_0}^{b}\left(\sqrt{\hbar^2k^2 - 2mV(\xi)}\right)d\xi - kb + \frac{\pi}{4}$$

At **large** k,

$$\delta_0(k) = \int_0^{\infty}\left(\sqrt{k^2 - 2mV(r)/\hbar^2} - k\right)dr$$

If we consider a k just below some special value (for instance k_1) then the wavefunction will rise in the classically forbidden region. However, when $k > k_1$, the wavefunction will have a node in the classically forbidden region and thus be of opposite sign once it is outside the barrier. Thus we see that the phase shift will increase by approximately π.

(e)

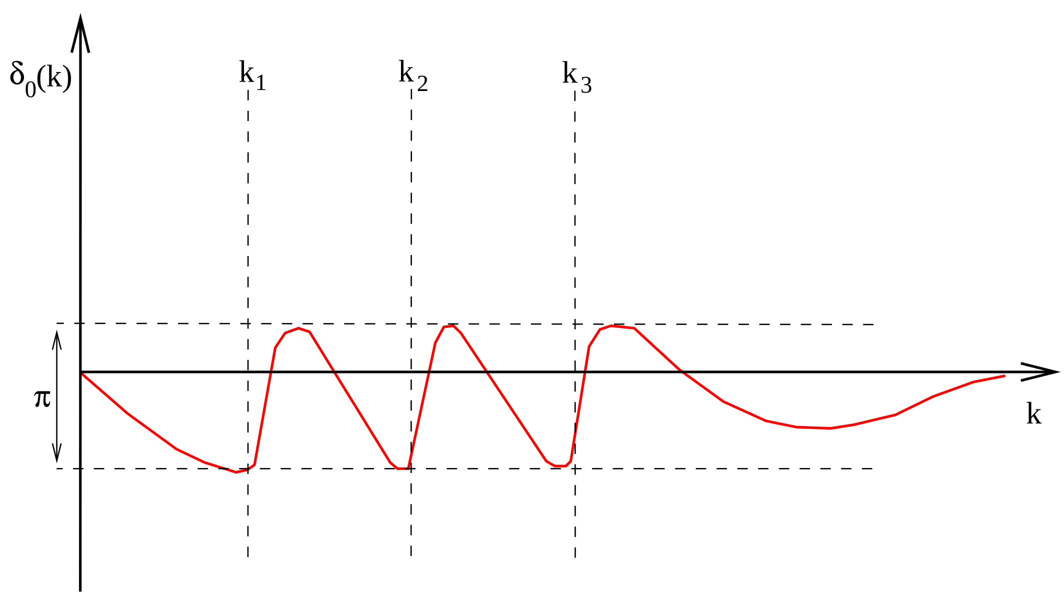

Figure 3: The s–wave phase shift as a function of k.

4. **p-wave phase shift**

(a) The wavefunction is spherical Bessel function

$$R(r) = j_1(qr) \qquad \text{for } r < b$$

$$R(r) = a_1 h_1^{(1)}(kr) + a_2 h_1^{(2)}(kr) \qquad \text{for } r > b$$

where $k = i\kappa$. In order to have a normalizable function,

$$R(r) = h_1^{(1)}(i\kappa r) = i\left(\frac{1}{\kappa r} + \frac{1}{\kappa^2 r^2}\right) e^{-\kappa r} \qquad \text{for } r > b$$

Imposing the necessary continuity of the wavefunction and its first derivative,

$$\frac{\sin(qb)}{q^2 b^2} - \frac{\cos(qb)}{qb} = C\left(\frac{1}{\kappa b} + \frac{1}{\kappa^2 b^2}\right) e^{-\kappa b}$$

$$\frac{2\cos(qb)}{qb^2} - \frac{2\sin(qb)}{q^2 b^3} + \frac{\sin(qb)}{b} = -C\left(\frac{1}{b} + \frac{2}{\kappa b^2} + \frac{2}{b^3 \kappa^2}\right) e^{-\kappa b}$$

From which

$$\sin(qb) = -Ce^{-\kappa b}$$

$$\frac{\cot(qb)}{qb} - \frac{1}{q^2 b^2} = \frac{1}{\kappa b} + \frac{1}{\kappa^2 b^2}$$

When a new bound state emerges, it is weakly bounded. Hence, its energy is $E \approx 0$. Thus we have $\cot(qb) \to \infty$ and

$$qb = n\pi \qquad n = 1, 2, \ldots$$

and since $U \approx q^2$, we have

$$U \approx \frac{n^2 \pi^2}{b^2} \qquad (\text{i.e. } \gamma = n\pi)$$

Thus in order to have one bound state

$$\pi \leq \gamma < 2\pi$$

(b) Given that b is a point outside the potential, for $r > b$

$$R_l(k, r) \propto a_l j_l(kr) + b_l n_l(kr)$$

which converges to

$$R_l(k, r) \xrightarrow{r\to\infty} \frac{a_l}{kr} \sin\left(kr - \frac{l\pi}{2}\right) - \frac{b_l}{kr} \cos\left(kr - \frac{l\pi}{2}\right)$$

$$= \frac{A}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l(k)\right)$$

where $\delta_l(k)$ is given by $\tan \delta_l(k) = -b_l/a_l$.

From continuity of the wavefunction and its derivative,

$$R_l(k, b) = a_l j_l(kb) + b_l n_l(kb)$$

$$\frac{\partial}{\partial r} R_l(k,b)\bigg|_{r=b} = a_l k \cdot j_l'(kb) + b_l k \cdot n_l'(kb)$$

Solving,

$$a_l = \frac{n_l R_l' - k n_l' j_l}{k n_l j_l' - k n_l' j_l}$$

$$b_l = \frac{j_l R_l' - k j_l' R_l}{k n_l' j_l - k j_l' n_l}$$

And thus

$$\tan\delta_l(k) = -b_l/a_l = \frac{j_l(x) R_l'(kb) - k j_l' R_l(k,b)}{n_l(x) R_l'(kb) - k n_l'(x) R_l(k,b)}$$

where $x = kb$. Using the following quantity,

$$\beta = \frac{b}{R_l(k,b)} \, \frac{\partial}{\partial r} R_l(k,b)\bigg|_{r=b}$$

we obtain the desired result

$$\tan\delta_l(k) = \frac{x j_l'(x) - j_l(x)\beta_l(k)}{x n_l'(x) - n_l(x)\beta_l(k)}$$

(c) For the p–wave

$$R_l(k,r) \propto j_1(\sqrt{k^2+U}r)$$

Hence,

$$\frac{\partial}{\partial r} R_l(k,b)\bigg|_{r=b} = \sqrt{k^2+U} \cdot j_1'(b\sqrt{k^2+U}) = \sqrt{k^2+U} \cdot j_1'(\sqrt{x^2+\gamma^2})$$

Thus,

$$\beta_1(k) = \frac{\sqrt{x^2+\gamma^2}}{j_1(\sqrt{x^2+\gamma^2})} j_1'(\sqrt{x^2+\gamma^2})$$

and

$$\tan\delta_l(k) = \frac{x j_1'(x) j_1(\sqrt{x^2+\gamma^2}) - \sqrt{x^2+\gamma^2} j_1(x) j_1'(\sqrt{x^2+\gamma^2})}{x n_1'(x) j_1(\sqrt{x^2+\gamma^2}) - \sqrt{x^2+\gamma^2} n_1(x) j_1'(\sqrt{x^2+\gamma^2})}$$

Using

$$\sin^2(y) = \frac{\tan^2(y)}{1+\tan^2(y)}$$

we have the partial wave cross section

$$\sigma_1(k) = 12\pi \frac{\sin^2\delta_1(k)}{k^2}$$

which is plotted in Figure 4 for various γ's.

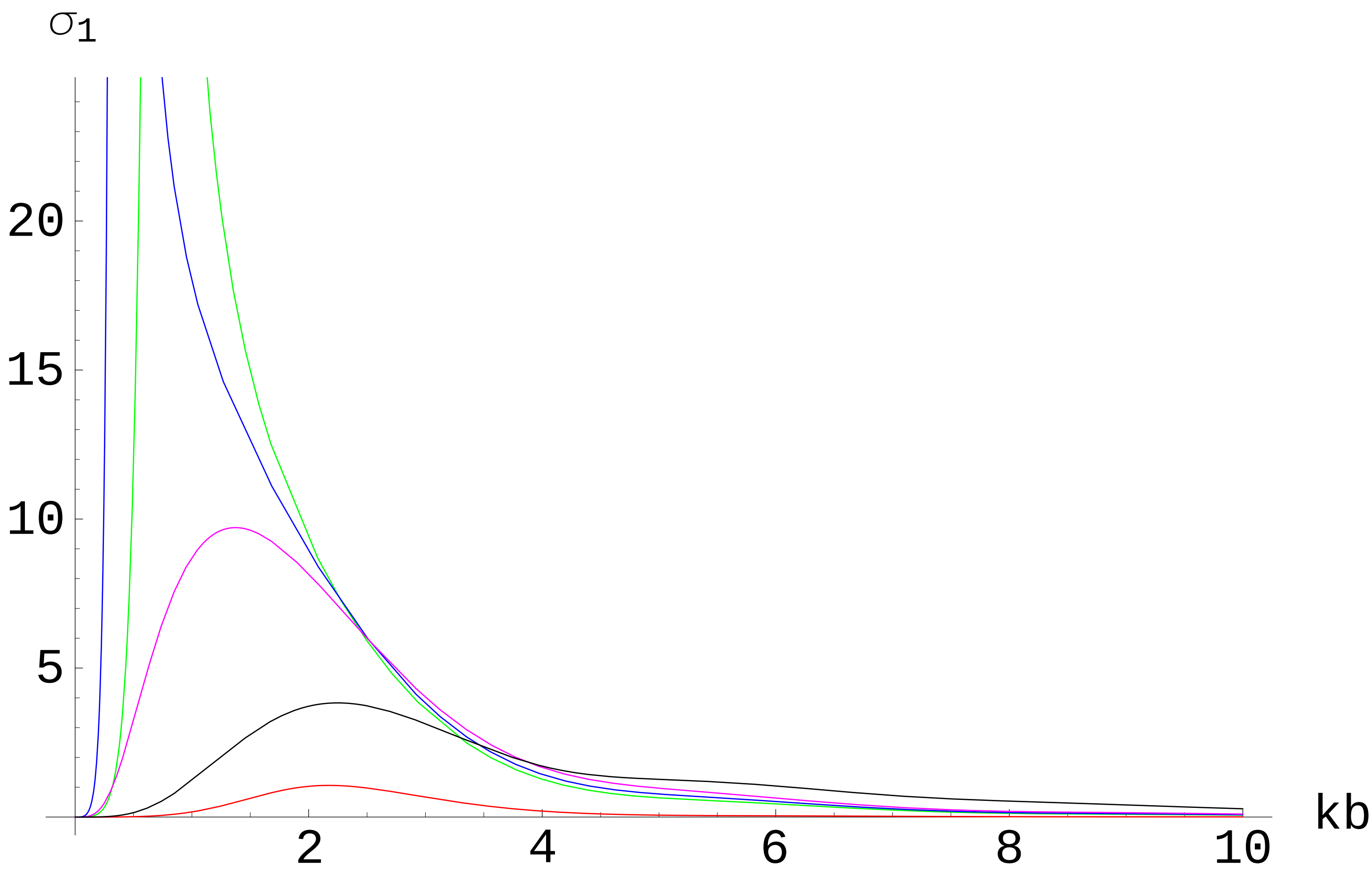

Figure 4: The partial wave cross section for $\gamma/\pi = 0.5,\ 0.93,\ 0.98,\ 1.05,\ 1.5$, red, green, blue, purple and black curves respectively. As we approach π, a sharp peak near $k = 0$ develops.

5. **The K-matrix**

(a) An adequate parametrization of a resonance

$$S_1(k) = \frac{k^2 - k_1^2 - ik\gamma_1}{k^2 - k_1^2 + ik\gamma_1}$$

with $\gamma_1 \ll k_1$.

The complex conjugate (for real k)

$$S_1(k)^* = \frac{k^2 - k_1^2 + ik\gamma_1}{k^2 - k_1^2 - ik\gamma_1}$$

and

$$S_1(k)^* S_1(k) = 1$$

i.e. $S_1(k)$ is unitary. The poles are at $k^2 - k_1^2 + ik\gamma_1 = 0$

$$k_\pm = -\frac{i\gamma_1}{2} \pm \sqrt{k_1^2 - \frac{\gamma_1^2}{4}}$$

on the complex k–plane. k_+ is near the physical region (see Figure 5).

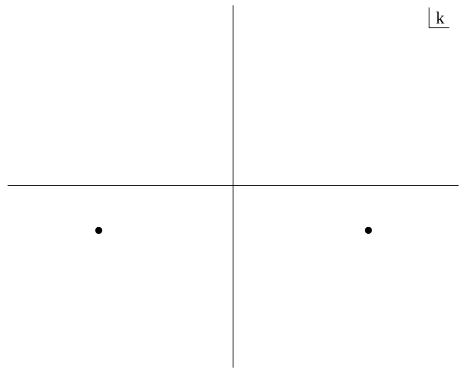

Figure 5: Poles on the k-plane.

Next,

$$S_1(k^2) = \frac{k^2 - k_1^2 - i\sqrt{k^2}\gamma_1}{k^2 - k_1^2 + i\sqrt{k^2}\gamma_1}$$

Because of the square root, k^2 lives on a Riemann surface. Its two sheets can be represented by a branch cut on the positive real axis along which the two sheets are glued together. The branch cut connects the branch point zero and "the point at infinity". The two poles $k_\pm$ are now at

$$k_\pm^2 = \left(k_1^2 - \frac{\gamma_1^2}{2}\right) \mp i\gamma_1\sqrt{k_1^2 - \frac{\gamma_1^2}{4}}$$

both located on the second sheet (see Figure 6).

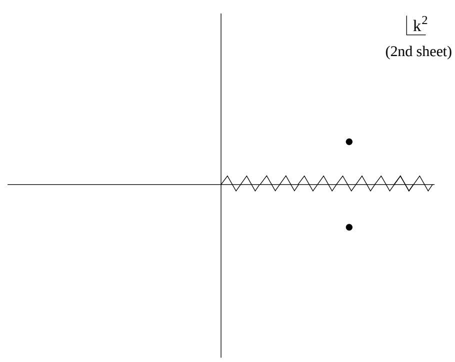

Figure 6: Poles on the k^2-plane.

A general S–matrix is expected to be single–valued as a function of real k. S has no poles in the upper–half plane (except possibly on the positive imaginary axis). Hence, the given S_1 is consistent with the general restrictions.

(b) Suppose

$$S_k(k) = \frac{k^2 - k_1^2 - ik\gamma_1}{k^2 - k_1^2 + ik\gamma_1} + \frac{k^2 - k_1^2 - ik\gamma_2}{k^2 - k_1^2 + ik\gamma_2}$$

If $k > 0$,

$$S_k(k)^* S_k(k) = 2\left[1 + \frac{((k^2-k_1^2)(k^2-k_2^2) + k^2\gamma_1\gamma_2)^2 - k^2(\gamma_1(k^2-k_2^2) - \gamma_2(k^2-k_1^2))^2}{((k^2-k_1^2)(k^2-k_2^2) + k^2\gamma_1\gamma_2)^2 + k^2(\gamma_1(k^2-k_2^2) - \gamma_2(k^2-k_1^2))^2}\right]$$

which is in general

$$S_k(k)^* S_k(k) \neq 1$$

(c) Under the K–matrix parametrization,

$$\begin{aligned}
\lim_{r\to\infty} u(r) &\propto \sin(kr) + kK(k)\cos(kr) \\
&= \frac{e^{ikr} - e^{-ikr}}{2i} + kK(k)\left(\frac{e^{ikr} - e^{-ikr}}{2}\right) \\
&\propto (1 + ikK(k))e^{ikr} + (-1 + ikK(k))e^{-ikr} \\
&\propto e^{-ikr} - \frac{1 + ikK(k)}{1 - ikK(k)} e^{ikr}
\end{aligned}$$

from which we see that

$$S(k) = \frac{1 + ikK(k)}{1 - ikK(k)}$$

Then, for any real k and $K(k)$,

$$S(k)^* S(k) = \left(\frac{1 - ikK(k)}{1 + ikK(k)}\right)\left(\frac{1 + ikK(k)}{1 - ikK(k)}\right) = 1$$

Thus, $S(k)$ is unitary.

As a function of k^2

$$S(k^2) = \frac{1 + i\sqrt{k^2}K}{1 - i\sqrt{k^2}K}$$

and if K is analytic, S has the expected branch cut.

(d) Recall that for a resonance

$$S_1(k) = \frac{k^2 - k_1^2 - ik\gamma_1}{k^2 - k_1^2 + ik\gamma_1} = \frac{1 + ik\frac{\gamma_1}{k_1^2 - k^2}}{1 - ik\frac{\gamma_1}{k_1^2 - k^2}}$$

Thus,

$$K_1(k) = \frac{\gamma_1}{k_1^2 - k^2}$$

For two resonances, we expect

$$K_2(k) = \frac{\gamma_1}{k_1^2 - k^2} + \frac{\gamma_2}{k_2^2 - k^2}$$

This gives

$$S_2(k) = \frac{(k_1^2 - k^2)(k_2^2 - k^2) + ik(\gamma_1(k_2^2 - k^2) + \gamma_2(k_1^2 - k^2))}{(k_1^2 - k^2)(k_2^2 - k^2) - ik(\gamma_1(k_2^2 - k^2) + \gamma_2(k_1^2 - k^2))}$$

$S_2(k)$ has poles at

$$\pm k_1 \qquad \text{and} \qquad \pm\, k_2$$

For $k^2 \approx k_j^2$, the denominator of S_2 has the form

$$1 - \frac{ik\gamma_j}{k_j^2 - k^2} + \ldots \propto k_j^2 - k^2 - i\gamma_j k$$

which is the resonance.

(e) Making a Taylor expansion

$$K(k) = c_1 + c_2 k^2 + \ldots$$

To have a bound state, S should have a pole on the imaginary k–axis. For weakly bound (or virtual) state, the pole must be at small $|k|$. Since

$$S(k) = \frac{1 + ik(c_1 + c_2 k^2 + \ldots)}{1 - ik(c_1 + c_2 k^2 + \ldots)}$$

the condition on c_1 is

$$c_1 \to \pm\infty$$

Here the minus sign is for the bound state and plus is for the nearly bound virtual state.

Now by definition,

$$\lim_{r\to\infty} u(r) \propto \sin(kr) + kK(k)\cos(kr)$$
$$= (1 + ikK(k))e^{ikr} + (-1 + ikK(k))e^{-ikr}$$

Suppose c_1 is large and negative. Then, for $k = i\kappa$,

$$\lim_{r\to\infty} u(r) \propto (1 - \kappa c_1)e^{-\kappa r} + (-1 - \kappa c_1)e^{\kappa r}$$

We have a bound state if

$$\lim_{r\to\infty} u(r) \propto e^{-\kappa r}$$

from which

$$\kappa c_1 = -1$$