B.2.2. APPLICATIONS & EXAMPLES

The applications of scattering theory are legion in physics - particularly in particle physics (most experiments are scattering experiments) and in areas where scattering is important (condensed matter physics, astrophysics, chemical physics, etc..). In what follows we hardly touch the surface of this - our main task is to look at a few simple but quite general features of scattering off both potential wells & potential barriers, and then to explicitly calculate these for a few specific models.

B.2.2 (a) BOUND STATES, POLES, & RESONANCES

If we change a potential $V(r)$ from a repulsive to an attractive one, then the spectrum of the system undergoes a radical change - from extended states for a repulsive potential, to a sum of positive energy extended states, and negative energy bound states, for an attractive potential.

However the details depend on the dimension of the system. In fact the following general results are true:

- In 3d, the strength $|V|$ of the attractive potential has to be finite before a bound state appears - thus there is a critical strength required for this.
- In 2d, an arbitrarily weak attractive potential will give a bound state - the critical strength is zero. The energy of the bound state E_b is given by

$$E_b \sim -\epsilon_0 \exp(-\epsilon_0/\bar{V}) \qquad (2d) \qquad (326)$$

where ϵ_0 is the energy scale determined by the spatial extent of the well (via the uncertainty principle); and so we see that the energy of the bound state is exponentially small in $\bar{V}$.

- In 1d, the critical strength is again zero, but now we have

$$E_b \sim -\epsilon_0 \left(\bar{V}/\epsilon_0\right)^n \qquad (1d) \qquad (327)$$

where the exponent n is typically 2. Thus in 1d the bound state energy is a power of $\bar{V}$.

Whatever is the dimension, it is clear that the scattering functions and the S-matrix will have to have some sort of singular behaviour as a function of energy (or of k^2) at the critical energy.

I will not attempt here to give a general discussion for arbitrary potentials, which is the sort of thing that mathematicians do. The argument for a finite critical strength V_c in 3d was already given above (cf eqtn (318)), and consists in showing that in 3d, the kinetic energy always exceeds $|\bar{V}|$ for small $\bar{V}$. The 1d and 2d cases need a closer look, since the Born approximation fails there.

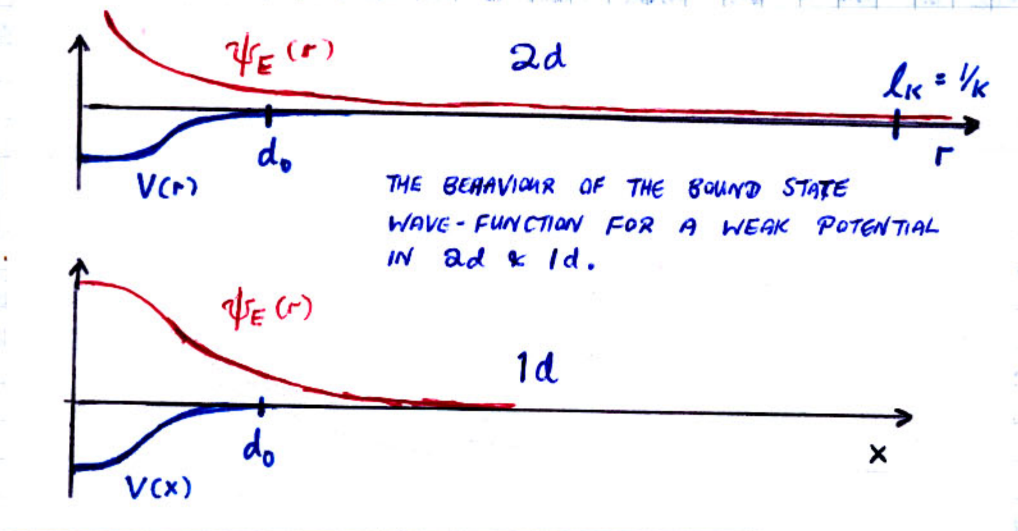
<u>2-d Bound States</u>: Suppose we have a potential $V(r)$, such that $V(r) \to 0$ for $r > d_0$, and $V(r) < 0$ for $r < d_0$. We assume a typical strength $\bar{V}$, ie we assume that

$$\int d^2r\, V(r) = 2\int_0^\infty r\,dr\, V(r) = -\bar{V} d_0^2 \qquad (328)$$

The 2-d Schrodinger eqtn is then, for this $l=0$ bound state:

$$\left[\frac{-\hbar^2}{2m}\left(\frac{1}{r}\partial_r\, r\partial_r\right) + \left(V(r)-E\right)\right]\psi(r) = 0. \tag{329}$$

Now since we already know that $|\bar{V}| \gg E$, we can drop E from this eqtn, in the region where the potential is important. Thus we wish to match the soltns between the far regime, where $r \gg d_0$, and the regime inside the potential well.



THE BEHAVIOUR OF THE BOUND STATE WAVE-FUNCTION FOR A WEAK POTENTIAL IN 2d & 1d.

In the regime far from the potential well we solve (329) with $V(r)=0$. This has to be a Hankel function of imaginary argument (the momentum in the 2d Green function of (263) is now $\tilde{k} = ik$), often called a MacDonald function - one has

$$K_\mu(z) = \frac{\pi}{2}\, e^{i\frac{\pi}{2}(\mu+1)} H^{+}_{\mu}(iz) \tag{330}$$

and the solution for the Green function for negative energy, generalising (263), is

$$G_0(r-r';E) \xrightarrow[E<0]{} \frac{2m}{\hbar^2}\,\frac{-1}{2\pi}\,K_0(\tilde{k}|r-r'|) \qquad (2d) \tag{331}$$

which has the asymptotic properties

$$G_0(r,E) \xrightarrow[E<0]{} \left.\begin{cases} \dfrac{2m}{\hbar^2}\,\dfrac{-1}{(8\pi\tilde{k}r)^{1/2}}\,e^{-\tilde{k}r} & (kr \gg 1) \\[2ex] \dfrac{2m}{\hbar^2}\,\dfrac{1}{2\pi}\,\ln\left(\dfrac{C_1\tilde{k}r}{2}\right) & (kr \ll 1) \end{cases}\right\} (2d) \tag{332}$$

(compare (264)), where of course

$$\tilde{k}^2 = \frac{2m}{\hbar^2}|E| \tag{333}$$

with $E<0$.

We now see that there are 2 length scales in the problem; the scale $l_{\tilde{k}} = 1/K$, and d_0; and l_K is exponentially larger than d_0.

Suppose we now integrate the Schrodinger eqtn up to a length scale r_0 which is outside the potential, but still much less than $1/K$, so that we can ignore the term $E\psi$ in the integration. Then we have

$$\frac{\hbar^2}{2m}\,\partial_r\psi\Big|_{r=r_0} = \frac{1}{r_1}\int_0^{r_1} dr\, V(r) = \frac{1}{2r_1}\bar{V}d_0^2 \tag{334}$$

and if now match derivatives at a distance $\sim d_0$, we get, using the behaviour of the solution in (332) outside the potential, that

$$\frac{\hbar^2}{2m}\frac{1}{d_0 \ln \tilde{\kappa} d_0} \sim \frac{1}{d_0}\int_0^{d_0} r\,dr\, V(r) \sim \bar{V} d_0 \qquad (335)$$

so that we have a solution for $E_b = -\hbar^2\tilde{\kappa}^2/2m$ given by

$$\left.\begin{aligned} E_b &\sim \frac{\hbar^2}{md_0^2}\exp\left\{-\frac{\hbar^2}{m}\frac{1}{\int r\,dr\,|V(r)|}\right\} \\ &\sim -\epsilon_0 \exp\left\{-\epsilon_0/|\bar{V}|\right\} \end{aligned}\right\} \qquad (336)$$

We will see, in discussing examples, how this works out in practise. Note how extremely slowly the wave-function decays with r outside the potential well - the particle spends virtually all its time far from the well.

<u>1-d Bound states</u>: We have already looked at an example of 1-d bound states, in the context of the δ-function and sech^2 potential wells. (pp. 93-97). Thus I will be brief here. The Schrodinger eqtn is

$$\left(-\frac{\hbar^2}{2m}d_x^2 + (V(x) - E)\right)\psi(x) = 0 \qquad (337)$$

Outside the well, the wave function has the form: $\psi(x) \sim e^{-\tilde{\kappa}x}$ (338)

Following through the same kind of development as above, we get a matching eqtn of form

$$\frac{\hbar^2}{2m}\kappa = -\int_{-\infty}^{\infty} dx\, V(x) \qquad (339)$$

so that the bound state energy is

$$\left.\begin{aligned} E_b &= -\frac{m}{2\hbar^2}\left[\int dx\, V(x)\right]^2 \\ &= -\bar{V}^2/\epsilon_0 \end{aligned}\right\} \qquad (340)$$

in line with eqtn (327).

<u>ANALYTICITY OF SCATTERING FNS</u>: Now let's consider how both the scattering of positive energy states, and the formation of bound states at negative energies, must affect the analytic behaviour of the S-matrix. It is useful to begin by considering the simple 1-d case, to give us a feeling for how things work, before discussing the general case. We recall (cf eqtns. (272)-(276), and (300)) that we can write the S-matrix in 1-d in the

simple form

$$S_k = \frac{k - ig_k}{k + ig_k} = \frac{1 + i\tan\delta_k}{1 - i\tan\delta_k} \qquad (341)$$

For the simple δ-function potential, this phase shift is: $\tan\delta_k \to -g_0/k$ (342)

Now consider how this function behaves when we have potential well, for the δ-fn potential. Writing it as

$$\left.\begin{aligned} S_k &= \frac{k - ig_0}{k + ig_0} \qquad (g_0 > 0) \\ \text{and} \quad S_k &= \frac{k + i|g_0|}{k - i|g_0|} = \frac{k + i\left(\frac{2m}{\hbar^2}\right)^{1/2}\bar{\kappa}}{k - i\left(\frac{2m}{\hbar^2}\right)^{1/2}\bar{\kappa}} \qquad (g_0 < 0) \end{aligned}\right\} \quad (343)$$

We can also write this as a function of energy E; then we have

$$\left.\begin{aligned} S(E) &= \frac{\sqrt{E} - i(\hbar^2/2m)^{1/2} g_0}{\sqrt{E} + i(\hbar^2/2m)^{1/2} g_0} \qquad (g_0 > 0) \\ S(E) &= \frac{\sqrt{E} + i(\hbar^2/2m)^{1/2}|g_0|}{\sqrt{E} - i(\hbar^2/2m)^{1/2}|g_0|} = \frac{\sqrt{E} + i\kappa}{\sqrt{E} - i\kappa} \qquad (g_0 < 0) \end{aligned}\right\} \quad (344)$$

Looking at (343), we see that there is a simple pole in the S-matrix at $k = i|g_0|$, which signals the existence of the bound state. If we let $k \to 0$, we also see that $S_k \to -1$; we come to this below.

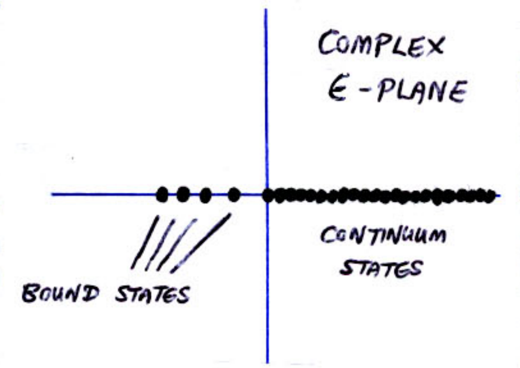
Looking at (344), we see that not only does $\sqrt{E}$ have a pole at $i\kappa$ (also signifying the bound state), but also E has a branch cut - this corresponds to the continuum of positive energy states.

These are simple examples of an interesting general feature of the scattering functions, viz., that their properties are determined, as a function of energy E or momentum $k = (2mE/\hbar^2)^{1/2}$, by the singularities (poles, branch cuts) of these functions in the complex E (or k) planes. This is of course obvious, since we know we are dealing with complex functions in the complex plane - but it is interesting and important to see where these poles and branch cuts are, and how they then determine the behavior of $G(E)$, $S(E)$, $T(E)$, $K(E)$, etc.

To see how this works let's consider again the Green function operator $\hat{G}(E)$, which we write now as

$$\left.\begin{aligned} \hat{G}(E) &= |n\rangle \frac{1}{E - \hat{H}} \langle n| \\ &= |n\rangle\langle n| \frac{1}{E - \hat{H}} |n\rangle\langle n| = |n\rangle \frac{1}{E - E_n} \langle n| \end{aligned}\right\} \quad (345)$$

where the states $|n\rangle$ are now the exact eigenstates of the full Hamiltonian $\hat{H}$, and we use the summation convention, summing over $|n\rangle$. It then follows that as a function of the complex energy ϵ, we must have for our scattering problem the kind of analytic structure shown in the diagram below. The Green function has simple poles for every one of the eigenstates $|n\rangle$, at energies $E = E_n$. These divide into a continuum of "free" states (ie, delocalised states extending out to infinite range), plus a finite set of discrete modes, corresponding to bound states.



The continuum of poles corresponding to the positive energy extended states can be treated as a branch cut - it is easy to see that the magnitude of the branch cut $A(E)$, at positive energy E, is related to the density of poles $N(E)$ (ie., the density of states) by

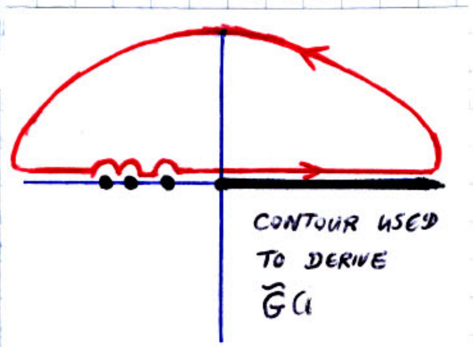
$$N(\epsilon) = \frac{-1}{\pi} A(\epsilon) \tag{346}$$

(the jump in $G(\epsilon)$ on crossing through a pole is $-2\pi i$, whereas the jump in crossing the branch cut is $2iA(E)$). These are the only singularities of $G(E)$. It then follows that we can define a function

$$\tilde{G}(\epsilon) = G(\epsilon) - G(\infty) \tag{347}$$

and, provided $\tilde{G}(\epsilon)$ falls off sufficiently fast as $|E| \to \infty$, we can write, using Cauchy's theorem, that

$$\tilde{G}(\epsilon) = \frac{1}{2\pi i} \oint dz \, \frac{\tilde{G}(z)}{\epsilon - z} \tag{348}$$



$$\begin{aligned} &\longrightarrow \sum_{n \in n_B} \frac{1}{\epsilon - E_n} + \frac{1}{\pi} \int_0^\infty dx \, \frac{\mathrm{Im}\, \tilde{G}(x + i\delta)}{x - \epsilon} \\ &= \sum_{n \in n_B} \frac{1}{\epsilon - E_n} + \frac{1}{\pi} \int_0^\infty dx \, \frac{A(x)}{x - \epsilon} \end{aligned} \tag{349}$$

where we sum over states $n \in n_B$ (the bound states) & where ϵ can be anywhere in the complex plane, and to go from (348) to (349) we choose the contour shown in the figure. If we wish to find the energy dependence of $G(\epsilon)$ on the real axis, we let $\epsilon \to E + i\delta$, to then derive the function $G^+(E)$:

$$\tilde{G}^+(E) = \tilde{G}(\epsilon \to E + i\delta) = \sum_{n \in n_B} \frac{1}{E - E_n + i\delta} + \frac{1}{\pi} \mathbb{P} \int_0^\infty dx \, \frac{A(x)}{x - E} \tag{350}$$

where to get (350) we use the usual rule that for any function $f(z)$, vanishing as $z \to \infty$,

$$2\pi i f(\epsilon + i\delta) = \int_{-\infty}^{\infty} dx \, \frac{f(x)}{x - \epsilon - i\delta} = \mathbb{P} \int dx \, \frac{f(x + i\delta)}{x - \epsilon} + i\pi f(\epsilon) \tag{351}$$

(for which see mathematical supplements).

From the result in (350) for $\tilde{G}^+(E)$ we can derive the "Kramers-Kronig" relations for the Green function (PTO): Taking the real and imaginary parts of (350), we have

$$\left.\begin{aligned}\mathrm{Re}\, G^+(E) &= \sum_{n\in n_B} \frac{1}{E-E_n} + \frac{1}{\pi}\mathbb{P}\int_0^\infty dx\, \frac{\mathrm{Im}\, G^+(x+i\delta)}{x-E} \\ \mathrm{Im}\, G^+(E) &= -\pi\sum_{n\in n_B} \delta(E-E_n) - \frac{1}{\pi}\mathbb{P}\int_0^\infty dx\, \frac{\mathrm{Re}\, G^+(x+i\delta)}{x-E}\end{aligned}\right\} \quad (352)$$

These Kramers-Kronig relations are used throughout physics. They are actually a consequence of causality. The fact that we can close the contour in the upper half-plane, as shown, assumes there are no other poles in this plane. But we can prove this as follows. Since cause cannot antecede effect, the function

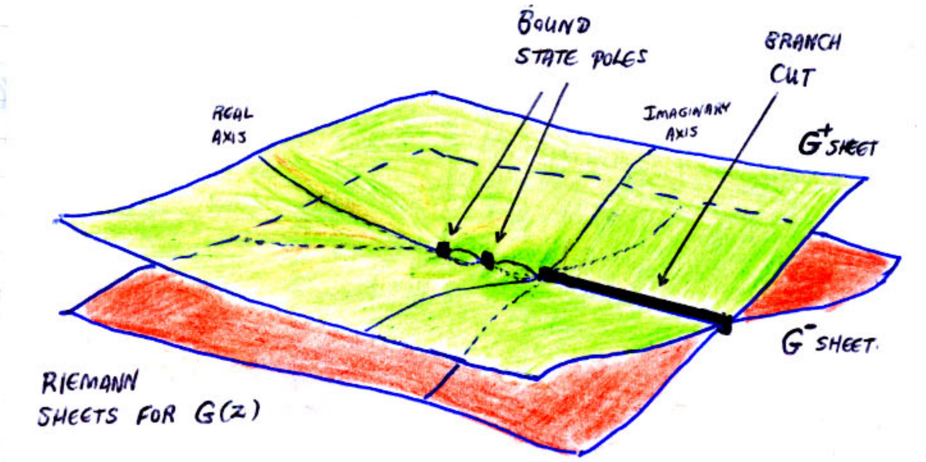
$$G(t) = 0 \qquad (t<0) \tag{353}$$

Now writing

$$G(\epsilon) = \int_{-\infty}^{\infty} dt\, e^{i\epsilon t}\, G(t) \longrightarrow \int_0^\infty dt\, e^{i\epsilon t}\, G(t) \tag{354}$$

for complex ϵ, we see that this function $G(\epsilon)$ can have no singularities for $\mathrm{Im}\,\epsilon > 0$.

It now makes sense to define a function $G(z)$, existing on the extended multi-sheeted complex plane as shown in the figure below. We have typically a 2-sheeted structure, and as is typical in this case, passing through the branch cut on some contour takes us from one sheet to the other. The convention then is to assume that one of these sheets describes the retarded function $G^+(z)$, and the other describes the advanced function $G^-(z)$. This multi-sheeted structure is of course necessary if we are to make sense of $G(z)$ as a complex variable.



RIEMANN SHEETS FOR $G(z)$

We note that since the functions $G(E)$, $S(E)$, and $T(E)$ are all linearly related to each other, they must all have the same singular structure (the same is not true of $K(E)$).

Now let us return to less abstract discussion, and make a few observations about the behaviour of the phase shifts in all of this. It is actually most useful, in a first look at this, to consider the 3d case, where we can make a clear intuitive connection to the scattering length. Consider therefore a short-ranged potential which can be either attractive or repulsive, and what will be the behaviour of both the phase shift and the scattering length in this problem, particularly in the limit $k\to 0$.

Before doing any calculations, let's just consider what the wave functions will look like around the potential, as a function of its strength. We write the radial function as

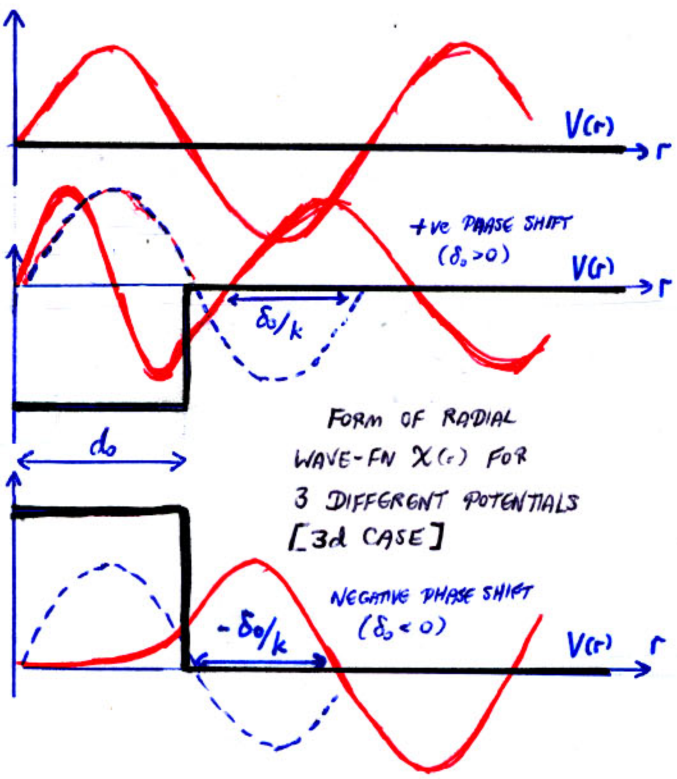
$$\psi_l(r) = r\,\chi(r) \tag{355}$$

so that

$$\chi''(r) + \left[\frac{2m}{\hbar^2}(E-V(r)) - \frac{1}{r^2}l(l+1)\right]\chi(r) = 0 \tag{356}$$

and so in the vicinity of the potential the wave-function looks as shown below. The effect of a attractive well is to pull the wave-function into the origin; a repulsive potential pushes it out. The form of the wave-fn for $E > 0$, outside the potential, is

$$\left.\begin{array}{l}\chi(r) \sim \sin(kr + \delta_0(k)) \\ \qquad\qquad (r > d_0)\end{array}\right\} \quad (357)$$



FORM OF RADIAL WAVE-FN $\chi(r)$ FOR 3 DIFFERENT POTENTIALS [3d CASE]

whereas inside the potential region, we have

$$\chi(r) = \begin{cases} \sin \tilde{k}r & (E > V_0 > 0) \\ \sinh \tilde{k}r & (V_0 > E > 0) \end{cases} \quad (358)$$

for the repulsive barrier, where $V_0 > 0$,

$$\tilde{k} = \left(\frac{2m}{\hbar^2}|E - V_0|\right)^{1/2} \quad (359)$$

On the other hand for the potential well, as soon as a bound state forms, at a bound state energy $E = -E_0$, we also get a bound state wave fn; outside the well we have:

$$\chi_0(r) \sim e^{-\kappa_0 r} \qquad \left(\kappa_0^2 = \frac{2m}{\hbar^2}|E_0|\right) \quad (360)$$

whereas inside the potential well we have

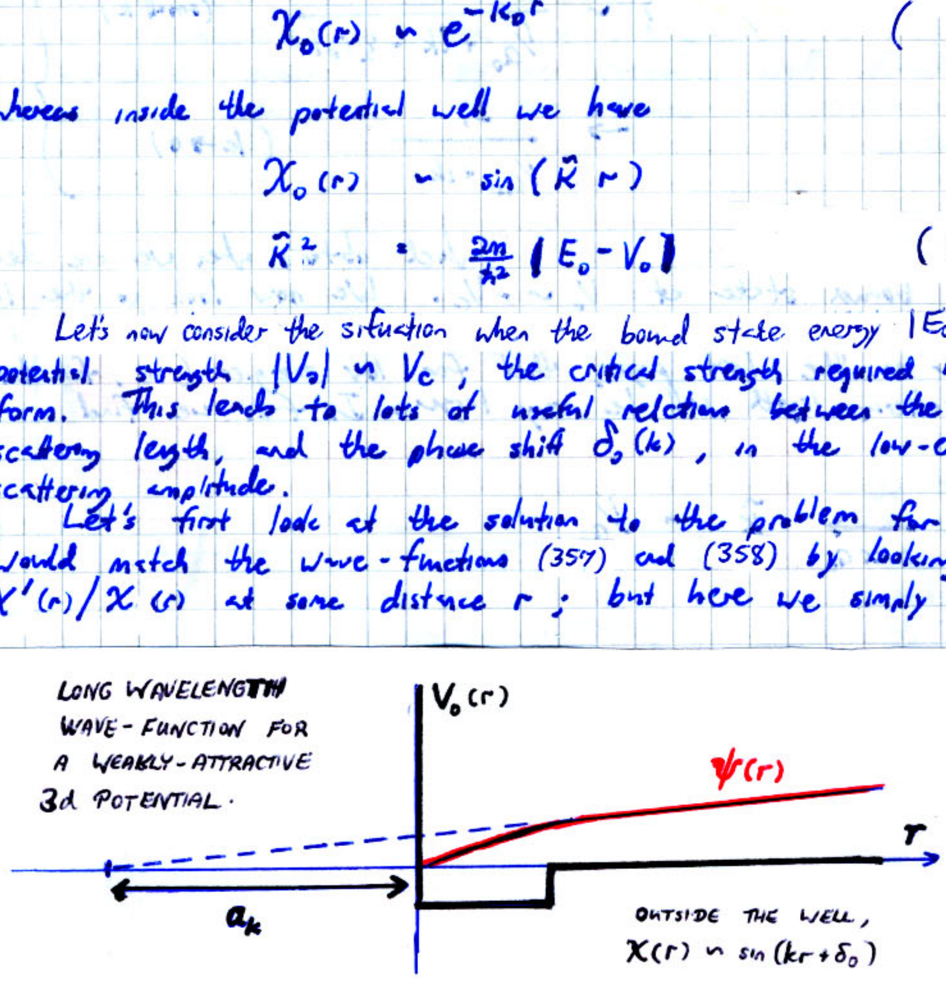
$$\chi_0(r) \sim \sin(\tilde{k} r) \quad (361)$$

$$\tilde{k}^2 = \frac{2m}{\hbar^2}|E_0 - V_0| \qquad (V_0 < 0) \quad (362)$$

Let's now consider the situation when the bound state energy $|E_0|$ is very small, ie., the potential strength $|V_0| \sim V_c$, the critical strength required in 3d for a bound state to form. This leads to lots of useful relations between the bound state energy, the scattering length, and the phase shift $\delta_0(k)$, in the low-energy ($k \to 0$) limit of the scattering amplitude.

Let's first look at the solution to the problem for small k. Normally we would match the wave-functions (357) and (358) by looking at the logarithmic derivative $\chi'(r)/\chi(r)$ at some distance r; but here we simply note that when k is very small, we have

$$\left.\begin{array}{l}\dfrac{\chi'(r)}{\chi(r)} \xrightarrow[kr \ll 1]{} k \cot \delta_0(k) \\ \qquad\qquad \sim -1/a_k\end{array}\right\} \quad (363)$$



where a_k is the intercept shown at left. Now it is actually easy to see that in the $k \to 0$ limit, the quantity a_k is nothing but the scattering length a_0 defined previously (cf eqtn (290)). For as we saw, in 3d,

$$\left.\begin{aligned} a_0 &= \lim_{k\to 0} |f_0(k)| = \lim_{k\to 0} \frac{1}{k}\left|\frac{1}{\cot\delta_0(k) - i}\right| \\ &= \lim_{k\to 0} a_k \end{aligned}\right\} \quad (3d) \qquad (364)$$

Thus we have a nice interpretation of the scattering length as the intercept, for small k, of the external wave-function with the real axis (see figure on last page). Note another equivalent way of defining a_k; from (363) we also have

$$\frac{d}{dk}\delta_0(k) \xrightarrow[\text{SMALL } k]{} -\frac{1}{a_k}\frac{\sin^2\delta_0(k)}{k^2} \equiv -a_k \qquad (3d) \qquad (365)$$

where we use (290) again. Thus a_k tells us the rate of change of phase shift with k in the small k limit.

For finite but small k it is very common to employ a phenomenological form for the scattering amplitude that uses these results. One writes

$$g_0(k) = k\cot\delta_0(k) \sim \left(\frac{-1}{a_0} + \frac{1}{2}r_0k^2\right) \qquad (366)$$

where $g_0(k)$ is the function in (253); thence

$$\left.\begin{aligned} f_0(k) &\sim \frac{-1}{1/a_0 + ik - \frac{1}{2}r_0k^2} \qquad (\text{small } k) \\ &\to \frac{-1}{1/a_0 + ik} \qquad (k\to 0) \end{aligned}\right\} \qquad (367)$$

Now let's look at the "threshold problem", which obtains when we are dealing with the onset of a bound state at $V_0 \sim -V_c$. We now look at the logarithmic derivative of the bound state wave-function, and match these at a distance $r \ll a_0$, noting from our picture on the last page, that for low energies (ie, for small k or small $\tilde{k}$) the scattering length will be very large. In fact we find

$$\frac{\chi_0'(r)}{\chi_0(r)} \xrightarrow[r \ll a_0]{} \tilde{k} \sim 1/a_0 \qquad (368)$$

so that we can also write that, for the bound state, for small k, that

$$\cot\delta_0(k) = -\tilde{k}/k = -\left(|E_0|/E\right)^{1/2} = -1/ka_0 \qquad (369)$$

with a scattering amplitude

$$f_0(k) \xrightarrow[k\to 0]{} \frac{-1}{\tilde{k} + ik} = \frac{-a_0}{1 + ika_0} \qquad (370)$$

and a scattering cross-section

$$\sigma_k^{Tot} \xrightarrow{\text{small } k} \frac{4\pi}{\tilde{k}^2 + k^2} = \frac{2\pi\hbar^2}{m}\frac{1}{E + |E_0|} \qquad (371)$$

Thus we reach the interesting conclusion that the appearance of the bound state is signalled by a divergence in the scattering cross-section as $k, E \to 0$. This is called THRESHOLD behaviour - it tells us that the onset of the bound state is seen in the divergence of the low-energy cross-section. We see also that as one approaches the threshold, $\delta_0(k)$ has very singular behaviour:

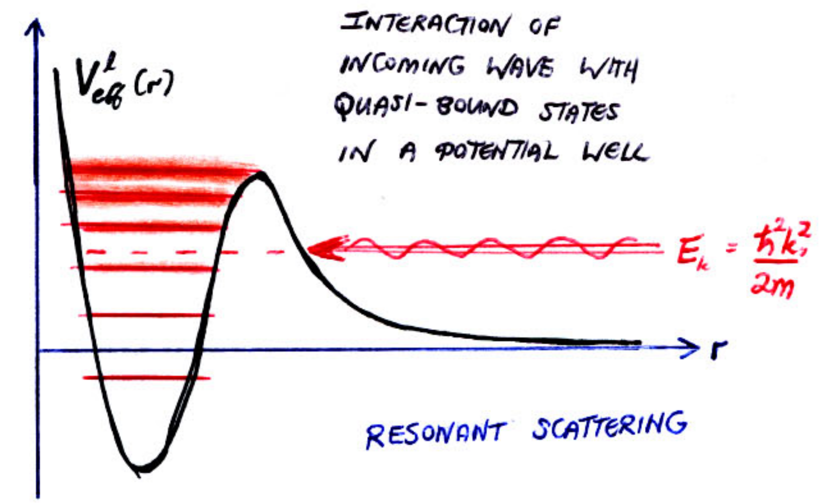
$$\left.\begin{array}{lll} \cot \delta_0(k) \xrightarrow[E \to 0]{} \infty & (|E_0| \text{ finite}) & \text{ie } \delta_0(k) \underset{k\to 0}{\to} 0 \\ \text{but} & & \\ \cot \delta_0(k) \xrightarrow[|E_0| \to 0]{} 0 & (E \text{ finite}) & \text{ie } \delta_0(k) \underset{|E_0| \to 0}{\to} (2n+1)\pi/2 \end{array}\right\} \quad (372)$$

Furthermore, we notice that by measuring the scattering cross-section as $k \to 0$, we can find the binding energy:

$$\lim_{k \to 0} \sigma_k^{Tot} = 4\pi a_0^2 = \frac{2\pi\hbar^2}{m} \frac{1}{|E_0|} \quad (373)$$

These remarkable results also have their counterparts in 2 dimensions, as we will see below.

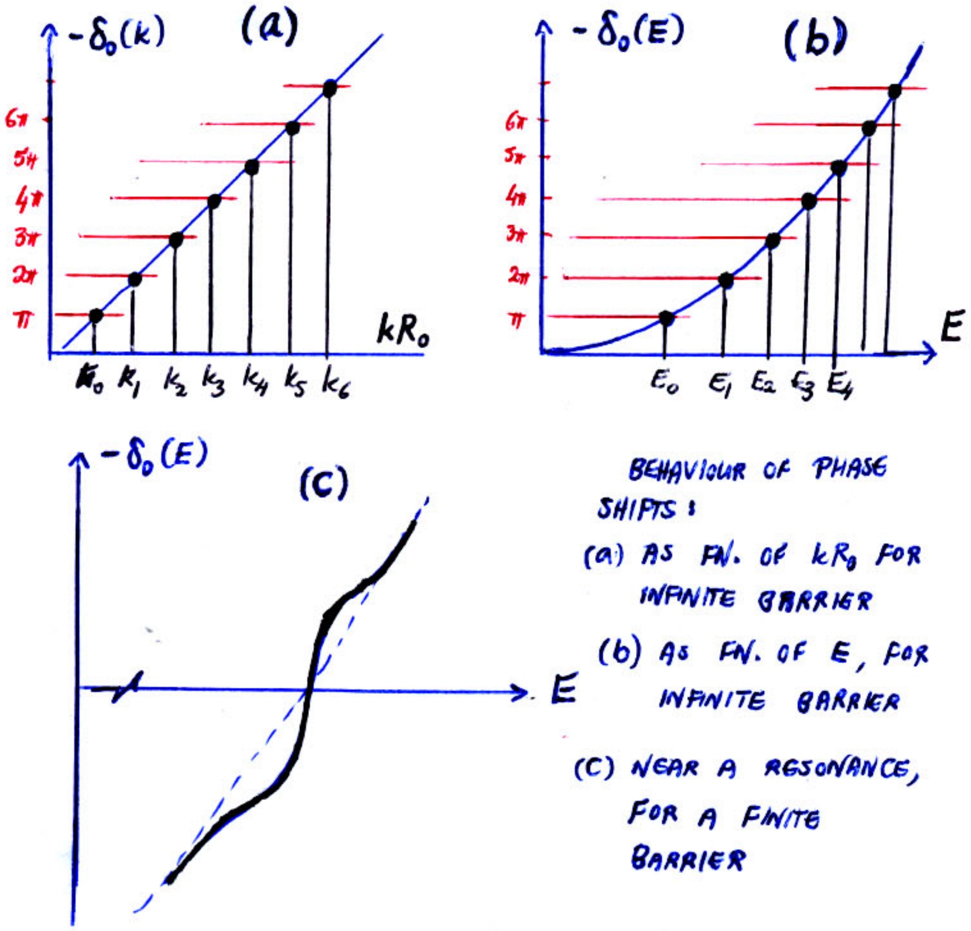
Finally, let's consider the phenomenon of RESONANCE. We already saw in our discussion of the 1d problem that the scattering amplitude can have interesting behaviour when some integer number of waves can fit into the potential at a given energy (cf p. 96, and eqtn (32)). This is a specific example of a more general phenomenon, arising when the scattered wave interacts with a state which is bound or quasi-bound by the potential well. Another example of the same is shown by the potential in the figure. Particles are incident upon an effective potential $V_{eff}(r)$, given by



RESONANT SCATTERING

$$V^{\ell}_{eff}(r) = \left\{\begin{array}{ll} V(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} & (3d) \\ V(r) + \frac{\hbar^2}{2m}\frac{\ell^2}{r^2} & (2d) \\ V(x) & (1d) \end{array}\right\} \quad (374)$$

so that any potential well at small r gives the form shown. We then wish to analyse the behaviour of the scattering amplitudes $f_\ell(k)$ and the phase shifts $\delta_\ell(k)$ as the energy $E_k = \hbar^2k^2/2m$ approaches the energy of the quasi-bound states inside the potential well. A clue to this is given already by the 1d problem discussed on p. 95-96; in that problem we saw that the transmission amplitude ($\propto$ here the scattering amplitude) oscillates as a function of incoming energy, with a period such that one oscillation occurs each time one passes through an "internal state" energy of the potential. Similar results are found when one looks at exactly solvable model potentials like those in the figure - we shall see an example below. In fact one finds the following general behaviour, as a function of the energy of the incoming particle:



BEHAVIOUR OF PHASE SHIFTS:

(a) AS FN. OF kR_0 FOR INFINITE BARRIER

(b) AS FN. OF E, FOR INFINITE BARRIER

(C) NEAR A RESONANCE, FOR A FINITE BARRIER

(i) If we imagine the case of an infinite potential barrier, then the bound states inside the barrier (assumed to be a δ-shell barrier of form

$$V(r) = V_0\,\delta(r-R_0) \tag{375}$$

with $V_0 \to \infty$) will occur at wave numbers such that

$$kR_0 = n\pi \tag{376}$$

Outside the barrier, we simply have

$$\delta_0(k) = kR_0 \tag{377}$$

(the external waves see the δ-shell as a hard sphere). We plot these results in Figs (a) and (b) at left.

However once we allow communication between the inside & outside, by tunneling through the barrier, things become quite different. The internal bound states become metastable, with line-broadening, and in the vicinity of the energy E_{ln} of the n-th quasi-bound state of the l-th angular momentum channel, we have

$$\cot\delta_l(E) = \cot\delta_l(E_{nl}) + \frac{2}{\Gamma_{nl}}(E-E_{nl}) + O(E-E_{nl})^2 \tag{378}$$

and since $\cot\delta_l(E_{nl}) = 0$ (379)

we have

$$\delta_l(E) = \delta_l^{(0)} + \tan^{-1}\frac{\Gamma_{nl}}{2(E-E_{nl})} \tag{380}$$

where we have defined the linewidth:

$$\Gamma_{nl} = \frac{-2}{\left.\frac{d}{dE}\cot\delta_l(E)\right|_{E=E_{nl}}} \tag{381}$$

and the phase shift $\delta_l^{(0)}$ is the phase shift far from the resonance. These eqns are telling us that the phase shift changes very rapidly, over a range a little less than π, over a narrow energy range $\sim \Gamma_{nl}$, where Γ_{nl} is the line-broadening of the quasi-bound state caused by its interaction with the plane-wave continuum. These results are equivalent to results for the S-matrix, the scattering function, and the scattering cross-section given by:

$$\left.\begin{aligned} S_l(E) &= S_l^{(0)} \frac{E - E_{nl} - i/_2 \Gamma_{nl}}{E - E_{nl} + i/_2 \Gamma_{nl}} \\ &= S_l^{(0)} \left[1 - \frac{i \Gamma_{nl}}{E - E_{nl} + i/_2 \Gamma_{nl}} \right] \end{aligned}\right\} \tag{382}$$

where the "bare" S-matrix is $$S_l^{(0)} = e^{2i\delta_l^{(0)}} \tag{383}$$

The scattering function is then, in 3d:

$$f_l(E) = f_l^{(0)} - \frac{1}{2k} \frac{\Gamma_{nl}}{E - E_{nl} + i/_2 \Gamma_{nl}} \qquad (3d) \tag{384}$$

with $f_l^{(0)}$ derived from $S_l^{(0)}$; and the scattering cross-section for 3d is

$$\sigma_l(k) = \sigma_l^{(0)} + \frac{4\pi}{k^2}(2l+1) \frac{\Gamma_{nl}^2/4}{(E - E_{nl})^2 + \Gamma_{nl}^2/4} \qquad (3d) \tag{385}$$

One can easily work out similar results for 1d and 2d problems. The upshot is that the scattering resonance is accompanied by a sharp peak in the cross-section, the inevitable consequence of the rapid passage of $\delta_l(E)$ through the resonant energy E_{nl}.

In scattering experiments on atoms or nuclei, such resonances are the sign of quasi-bound states. However one also sees them when a long-lived composite particle is created during high-energy collisions. At one time such resonances were viewed as a sign of unstable elementary particles (during the 1960's, in the heyday of "S-matrix theory").

B.2.2 (b) EXAMPLES IN 2 DIMENSIONS

There are innumerable examples in textbooks of 3d scattering, and thousands of papers on the topic. However in many ways 2d examples are more pedagogically useful, even though hardly discussed.

In what follows we look at the hard sphere, the soft sphere (and its limiting δ-fn form); the "2-d delta shell" potential, and the scattering off a flux tube. We will thereby see examples of all the behaviour described above.

PARTIAL WAVE EXPANSIONS : Let's begin with ordinary short-range potentials, and look at their scattering functions in partial wave expansion. The general solution to this problem was found already in section B.1.2(a). We have phase shifts

$$\delta_l(k) = \tan^{-1} \left\{ \frac{\beta_l(k) J_l(kr_0) - kr_0 J_l'(kr_0)}{\beta_l(k) Y_l(kr_0) - kr_0 Y_l'(kr_0)} \right\} \tag{386}$$

where the $\beta_l(k)$, given by $$\beta_l(k) = \frac{r}{R_l(kr)} \frac{d}{dr} R_l(kr) \Big|_{r=r_0} \tag{387}$$

are obtained by matching logarithmic derivatives at a distance r_0 outside the range of the potential.

Let's go quickly through the cases we've already seen:

(i) Hard Sphere: This is the simplest case. We recall that we deal here with the potential

$$V(r) = \left.\begin{matrix} \infty & (r < a_0) \\ 0 & (r > a_0) \end{matrix}\right\} \qquad (388)$$

with phase shifts given by

$$\delta_l(k) = \tan^{-1}\left(\frac{J_l(ka_0)}{Y_l(ka_0)}\right) \qquad (389)$$

(cf. eqtn. (128)). The high- and low-energy asymptotic forms of these phase shifts are just

$$\delta_l(k) \xrightarrow[ka_0 \gg 1]{} ka_0 - \frac{\pi}{2}(l + \tfrac{1}{2}) \qquad (390)$$

$$\delta_0(k) \xrightarrow[ka_0 \ll 1]{} \frac{\pi}{2\ln(C_1 ka_0/2)} \xrightarrow[ka_0 \to 0]{} 0 \qquad (391)$$

and where we ignore the higher-l phase shifts in the low-energy limit, since $\delta_l(k) \sim (ka_0)^{2l}$ for $l \neq 0$.

The low-energy properties are quite easy to obtain for this problem, from (391). One has, in the small k limit, that $\delta_0(k) \ll 1$, so we have

$$f_0(k) \sim \left(\frac{2}{\pi k}\right)^{1/2} \frac{\pi}{2\ln(C_1 ka_0/2)} \qquad (ka_0 \ll 1) \qquad (392)$$

and so the scattering cross-section is just

$$\left.\begin{aligned} \sigma_k^{Tot} &= 2\pi|f_0(k)|^2 \\ &\sim \frac{\pi^2}{k} \frac{1}{[\ln(C_1 ka_0/2)]^2} \xrightarrow[ka_0 \to 0]{} \infty \end{aligned}\right\} \qquad (393)$$

Thus we have the striking result that even though the phase shift for the 2-d hard sphere goes to zero in the long-wavelength limit, nevertheless the scattering cross-section goes to infinity (and so does the scattering amplitude $f_0(k)$)! The reason for this is quite simple. Even though the phase shift is going to zero, the wavelength $\lambda = 2\pi/k$ of the scattering wave is going to ∞. Since the scattering length here is just (cf (290), (363), and the figure on p. 145):

$$\left.\begin{aligned} a_k \xrightarrow[ka_0 \ll 1]{} -\frac{d}{dk}\delta_0(k) = \frac{1}{k}\delta_0(k) &= \sigma_k^{Tot}/2\pi \\ &= \frac{\pi}{2k} \frac{1}{[\ln(C_1 ka_0/2)]^2} \end{aligned}\right\} \qquad (394)$$

it goes to ∞ rather fast. For σ_k^{Tot} to remain finite as $k \to 0$, we would have required that $\delta_0(k) \sim O(k)$ in the long-wavelength limit. This does not happen because, as we have seen, in 2d the potential is not a small perturbation in the long-wavelength limit, and in fact the log form in (391) comes from the same form in the long-wavelength limit of the 2d Green function in (264) and (332).

One can also derive, from (390), the short-wavelength behaviour of the scattering amplitude and cross-section. However this turns out to be mathematically quite complex, so we will eschew it here.

(ii) Delta-function Potential : Here we will consider both the repulsive and the attractive case, ie, we consider

$$V(r) = \lim_{a_0 \to 0} \frac{V_0}{\pi a_0^2} \theta(d_0^2 - r^2) = V_0 \delta(r) \qquad (395)$$

with V_0 having either sign.

Consider first the repulsive case. Now, from eqtn (137), we know that we have

$$\delta_0(k) = \tan^{-1}\left(\frac{\pi}{2} \frac{1}{\ln(C_1 k d_0 / 2)} \right) \xrightarrow[d_0 \to 0]{} 0 \qquad (396)$$

Even when d_0 is still finite but very small, it only makes sense to consider the case where $kd_0 \ll 1$. We then see that the behaviour of this system is very interesting - it is exactly the same as the hard sphere in the long-wavelength limit!

Thus we see that we need to handle a δ-function potential with extreme care in 2d. The naive result, that because $\delta_0(k) = 0$, therefore the scattering cross-section is zero, is flat wrong.

Now consider the attractive problem, with $V_0 < 0$. This is a little delicate, so we do it in 2 different ways. First, here, we redo the calculation of (336), and then redo the calculation of the wave function & energy directly. Then, below, we calculate the T-matrix directly, using the Green function.

Let's first redo the calculation of (336). The formula (336) is not terribly transparent, since both E_0 and $\bar{V}$ diverge. So let's redo the calculation specifically for the δ-fn potential. We have to now match derivatives at the edge of the δ-fn., at a radius d_0 (which we keep finite but very small). Thus we have to match $\partial_r \psi$ at $r = d_0 - \epsilon$ with $\partial_r \psi$ at $r = d_0 + \epsilon$.

To get the former we simply integrate the Schrodinger eqtn, given by

$$\frac{1}{r}\partial_r \left(r \partial_r \right) \psi(r) = - \frac{2m}{\hbar^2} \frac{V_0}{\pi d_0^2} \theta(d_0^2 - r^2)\, \psi(r) \qquad (397)$$

from $r = 0$ to $r = d_0 - \epsilon$, to get

$$\frac{d_0}{\psi(d_0)} \partial_r \psi(r) \Big|_{r = d_0 - \epsilon} = \frac{2m}{\hbar^2} \int_0^{d_0 - \epsilon} r\, dr\, V(r) = - \frac{2m}{\hbar^2} \frac{V_0 d_0^2}{2\pi} \qquad (398)$$

where we assume here that $\psi'(r) \gg \psi(r)$ in the well, so that we can just treat it as a constant during the integration. Now consider the derivative just outside the potential well - we then have, assuming that $K_0^2 = 2m/\hbar^2 |E_0|$ is very small, and certainly that $\kappa_0 d_0 \ll 1$. Then we have

$$\frac{1}{\psi(r)} \partial_r \psi(r) \Big|_{r = d_0+\epsilon} = \frac{1}{d_0} \frac{1}{\ln(C_1 \kappa_0 d_0/2)} \qquad (399)$$

from (332). Equating (399) and (398), we get

$$\left.\begin{aligned} E_0 &= -\frac{\epsilon_0}{\pi C_1^2} \exp\left[-\epsilon_0/V_0\right] \\ \text{where} \quad \epsilon_0 &= 4\pi \frac{\hbar^2}{2m d_0^2} = 2\pi\hbar^2/m d_0^2 \end{aligned}\right\} \qquad (400)$$

Since ϵ_0 diverges as $d_0 \to 0$, we find that $|E_0| = 0$ for any V_0.

One can certainly be suspicious of some of the manoeuvres here (particularly those leading to (398). Thus we shall redo this problem more rigorously using the T-matrix method, below.

(iii) <u>Delta-Shell Potential</u>: This potential gives us a toy model for resonant scattering in 2d - the potential is:

$$V(r) = V_0 \delta(r - d_0) \qquad (401)$$

which we can write as a limiting case:

$$V(r) = \lim_{a_0 \to 0} \frac{V_0}{a_0} \theta(a_0 - 2|r - d_0|) \qquad (402)$$

Thus we have a circular barrier at a radius d_0, of infinite height and infinitesimal width, through which the particles must tunnel.

To solve this problem, we again use 2 methods. Here we will find the wave-function of the system, including the scattered wave, essentially using a Lippmann-Schwinger eqtn. Then, below, we will derive the T-matrix and f-function directly, using the integral eqtn for the T-matrix.

Consider the integral eqtn for the total wave-function, given again in real space by

$$\left.\begin{aligned} |\Psi^+(r)\rangle &= \phi_k(r) + \int d^2r' \, G_0^+(k, r - r') V(r') \Psi^+(r') \\ &= \phi_k(r) + \int d^2r' \, V(r') \frac{2m}{\hbar^2} \frac{-i}{4} H_0^+(k|r - r'|) \Psi^+(r') \end{aligned}\right\} (2d) \qquad (403)$$

A general attack on eqtns like this requires the theory of integral eqtns, which I will not assume here. Instead I will just use a particular technique from this theory. Suppose we We rewrite the bare Green function as an expansion over Bessel functions (this is a special case of eqtn (219) in part A). In the momentum representation we have

$$G_0^+(k, r - r') = \frac{2m}{\hbar^2} \int \frac{d^2q}{(2\pi)^2} \frac{e^{iq\cdot(r - r')}}{k^2 - q^2 + i\delta} \equiv \langle r|k\rangle G_0^+(k) \langle k|r'\rangle \qquad (404)$$

which we now write in the form

$$G_0^+(k, \underline{r}-\underline{r}') \quad = \quad \sum_l g_l^0(k, r-r') \, e^{il(\theta-\theta')} \quad \equiv \quad \langle r|l\rangle g_l(k,\theta\theta') \langle l|r'\rangle \qquad (405)$$

We can go between these 2 representations by noting the expansion of the plane wave in terms of Bessel fns, given already in (263):

$$\langle r|k\rangle \quad = \quad \sum_l i^l J_l(kr) \, e^{il\theta} \qquad (406)$$

from which we find that

$$g_l^0(k, r-r') \quad = \quad \frac{2m}{\hbar^2}\frac{1}{2\pi}\int_0^\infty q\,dq \, \frac{J_l(qr) J_l(qr')}{k^2 - q^2 + i\delta} \qquad (407)$$

To evaluate this integral, note it is even in q, so can be extended to $\int_{-\infty}^{\infty} dq$. Then contour integration gives us

$$g_l^0(k, r-r') \quad = \quad \frac{2m}{\hbar^2}\,\frac{-i}{4}\, H_l^+(kr_>) \, J_l(kr_<) \qquad (408)$$

where $r_> \equiv$ greater of r, r', and $r_<$ the lesser, ie

$$\left.\begin{aligned} r_> &= r\,\theta(r-r') + r'\,\theta(r'-r) \\ r_< &= r'\,\theta(r-r') + r'\,\theta(r-r') \end{aligned}\right\} \qquad (409)$$

and where we have done the integration by writing $J_l(qr') = \frac{1}{2}\left(H_l^+(qr') + H_l^-(qr')\right)$, and then noting that we have $H_l^\pm(z) \propto e^{\pm iz}$, so that we can close the integral contour in the upper/lower half-plane for $H^\pm(z)$ respectively.

If we rewrite the Lippmann-Schwinger eqtn in (403), by expanding the wave-fns in Bessel fns, as well, ie., writing $\phi_k(r)$ as in (406), and writing

$$\Psi^+(r) \quad = \quad \sum_l i^l \psi_l(kr) \, e^{il\theta} \qquad (410)$$

then we just have the integral eqtn

$$\psi_l(kr) \quad = \quad J_l(kr) \; + \int_0^\infty r'dr' \; g_l^0(k, r-r') \, V(r') \, \psi_l(kr) \qquad (411)$$

$$\left.\begin{aligned} &= J_l(kr) + \int_0^\infty r'dr' \, \frac{2m}{\hbar^2}\,\frac{-i}{4}\, H_l^+(kr_>) \, J_l(kr_<) \, V(r') \, \psi_l(kr) \\ &\equiv J_l(kr) - \frac{im}{2\hbar^2}\int_0^\infty r'dr' \, V(r')\,\psi_l(r') \Big[\theta(r-r') \, H_l^+(kr) J_l(kr') \\ &\qquad\qquad + \theta(r'-r) \, H_l^+(kr') J_l(kr)\Big] \end{aligned}\right\} \qquad (412)$$

This integral equation is still fairly formidable, but now we observe that for a potential like the Delta-shell potential or the Delta-function potential, it simplifies greatly, because the delta-fns collapse the integrals & we get algebraic eqtns.

Thus, for the delta-shell potential, we immediately see that we have the result:

$$\psi_{lk}(r) = J_l(kr) - \frac{im}{2\hbar^2} V_0 d_0 \psi_l(kd_0)\left[H_l^+(kr) J_l(kd_0)\,\theta(r-d_0) + H_l^+(kd_0) J_l(kr)\,\theta(d_0-r)\right] \tag{413}$$

and if we then set $r = d_0$, we get the result

$$\psi_{lk}(d_0) = \frac{J_l(kd_0)}{1 + \frac{im}{2\hbar^2} V_0 d_0 H_l^+(kd_0) J_l(kd_0)} \tag{414}$$

so that finally we have

$$\left.\begin{aligned}\psi_{lk}(r) = J_l(kr) - \frac{im}{2\hbar^2}\frac{V_0 d_0 J_l(kd_0)}{1 + \frac{im}{2\hbar^2} V_0 d_0 J_l(kd_0) H_l(kd_0)}\Big[&H_l^+(kr) J_l(kd_0)\,\theta(r-d_0)\\ &+ J_l(kr) H_l^+(kd_0)\,\theta(d_0-r)\Big]\end{aligned}\right\} \tag{415}$$

Now this result is very pretty perhaps but not really useful until we can extract the phase shifts from it. To do this we need to relate this solution to the scattered wave solution in terms of the f-function.

Let's first note that we can write the scattered wave as

$$\left.\begin{aligned}\Psi^+_{scatt}(r) &= \int d^2r'\, G_0^+(k, r-r') \langle r' | V | \Psi^+ \rangle\\ &= \frac{2m}{\hbar^2}\frac{-i}{4}\int d^2r'\, H_0^+(k|r-r'|)\, V(r')\, \Psi^+(r')\end{aligned}\right\} \tag{416}$$

(cf (303)), and that this is

$$\left.\begin{aligned}\Psi^+_{scatt}(r) &\xrightarrow[kr \gg 1]{} \frac{f_k(\theta)}{\sqrt{r}}\, e^{i(kr+\pi/4)}\\ &= \left(\frac{2}{\pi k r}\right)^{1/2} e^{i(kr+\pi/4)} \sum_l e^{i\delta_l(k)} \sin\delta_l(k)\, e^{il\theta}\end{aligned}\right\} \tag{417}$$

from (201) and (267). To equate these, we write the Green fn. in (416) in the separable form given by (405) and (408), to get

$$\left.\begin{aligned}\Psi^+_{scatt}(r) &= \sum_l \int d\theta' \int r'dr'\, \frac{2m}{\hbar^2}\frac{-i}{4} H_l^+(kr_>) J_l(kr_<)\, e^{il(\theta-\theta')}\, V(r')\, \Psi^+(r')\\ &\xrightarrow[kr \gg 1]{} \left(\frac{2}{\pi k r}\right)^{1/2} e^{i(kr+\pi/4)} \sum_l \frac{2m}{\hbar^2}\frac{-1}{4}\, e^{il\theta} \int r'dr'\, J_l(kr') V(r') \psi_{lk}(r')\end{aligned}\right\} \tag{418}$$

where we use the asymptotic behaviour of $H_l^+(z) = J_l(z) + iY_l(z)$ from (118), the definition of $\psi_l(kr)$ from (410), and assume that $r > r'$ for all important parts of the integration. Thus we find that

$$e^{i\delta_l(k)} \sin\delta_l(k) = \frac{2m}{\hbar^2}\frac{-1}{4}\int_0^\infty r\,dr\, J_l(kr) V(r) \psi_{lk}(r) \tag{419}$$

Substituting $\psi_{lk}(r)$ from (413) we then finally get that

$$e^{i\delta_l(k)} \sin \delta_l(k) = \frac{2m}{\hbar^2} \frac{-1}{4} \left[\frac{V_0 d_0 J_l^2(kd_0)}{1 + \frac{im}{2\hbar^2} V_0 d_0 J_l(kd_0) H_l^+(kd_0)} \right] \qquad (420)$$

and taking the imaginary part of this (using $H_l^+(kd_0) = J_l(kd_0) + i Y_l(kd_0)$) we get

$$\sin^2 \delta_l(k) = \frac{\frac{m}{2\hbar^2} V_0 d_0 J_l^2(kd_0)}{\left[1 - \frac{m}{2\hbar^2} V_0 d_0 J_l(kd_0) Y_l(kd_0)\right]^2 + \frac{m^2}{4\hbar^4} V_0^2 d_0^2 J_l^4(kd_0)} \qquad (421)$$

and one can also write useful forms for $\tan \delta_0$, etc.

It should now be obvious how one can do the same sort of thing for a δ-fn potential (indeed it is interesting to do this calculation again for a potential which is the sum of the Delta-shell potential we just did, and the δ-fn potential at the origin).

It should also be clear that the form of (420) just results from a geometric sum which comes from the multiple scattering in both the T-matrix and the Green fn.