Chapter 4. Resonances

Contents

This chapter is mainly summarized from the book by John R. Taylor, (*Scattering Theory*, John Wiley & Sons, (1992)).

1 1-D Square well problem - Bound and scattering states or continuum

Consider a particle with a mass of m in a one-dimensional square well potential,

$$V(x) = \begin{cases} \infty & ; \quad -\infty < x < 0 \\ -V_0 & ; \quad 0 < x < a \\ 0 & ; \quad a < x < \infty \end{cases}$$

The 1-D Schrödinger equation becomes

$$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)]\varphi(x) = E\varphi(x)$$

or

$$\varphi_{xx} = -K^2(x)\varphi$$

where

$$\begin{aligned} \frac{\hbar^2 K^2}{2m} &= E - V(x) \\ \varphi_x = \frac{\partial \varphi}{\partial x}, \qquad \varphi_{xx} &= \frac{\partial^2 \varphi}{\partial x^2} \end{aligned}$$

with the boundary conditions that

$$\begin{aligned} \varphi(0) &= 0 \\ \varphi(\infty) &\to \begin{cases} 0 & \text{(bound state)} \\ \text{sinusoidal ft} & \text{(unbound)} \end{cases} \end{aligned}$$

Another condition is that $\varphi(x)$ should be analytic (continuous and differentiable) in the whole region, that is, $\varphi(x)$ should be smoothly matched at $x = a$,

$$\frac{\varphi_x}{\varphi}|_{x<a} = \frac{\varphi_x}{\varphi}|_{x>a}$$

1.1 Discrete bound state problem, $E < 0$

If we write the interior and exterior wave functions as,

$$\begin{aligned} \varphi_I &= A \sin Kx, \quad \frac{\hbar^2 K^2}{2m} = V_0 - E \\ \varphi_E &= B \exp(-\kappa x), \quad \frac{\hbar^2 \kappa^2}{2m} = -E \end{aligned}$$

these boundary and matching conditions yield the dispersion relation (See Lecture II-5.)

$$K \cot Ka = -\kappa, \qquad \text{or} \qquad \eta = -\xi \cot \xi$$

where $\xi \equiv Ka$, $\eta \equiv \kappa a$. We further have

$$\rho^2 \equiv \frac{2mV_0 a^2}{\hbar^2} = \frac{2ma^2}{\hbar^2}(\frac{\hbar^2\kappa^2}{2m} + \frac{\hbar^2 K^2}{2m}) = \xi^2 + \eta^2$$

Graphically, the intersections of the curve $\eta = -\xi \cot \xi$ and the circle $\rho^2 = \xi^2 + \eta^2$ give the eigenenergies E_n. Note that there is no bound state for $\rho < \pi/2$, the ground state exists between $\frac{1}{2}\pi < \rho < \pi$, and there are n bound states for a given $(n - \frac{1}{2})\pi < \rho < (n + \frac{1}{2})\pi$.

1.2 Scattering state problem, $E > 0$

If we write the interior and exterior wave functions as,

$$\begin{aligned}\varphi_I &= A\sin Kx, \quad \frac{\hbar^2 K^2}{2m} = V_0 + E \\ \varphi_E &= B\sin(kx+\delta), \quad \frac{\hbar^2 k^2}{2m} = E\end{aligned}$$

then these boundary and matching conditions again determine δ (See Lecture IV-4.),

$$\begin{aligned}\tan\delta &= \frac{(k/K)\tan Ka - \tan ka}{1 + (k/K)\tan Ka \tan ka} \\ \delta &= \tan^{-1}(\frac{k}{K}\tan Ka) - ka\end{aligned}$$

The cross section becomes

$$\sigma = \frac{4\pi}{k^2}\sin^2\delta$$

Low energy behavior: At very low energies, we get

$$\begin{aligned}\tan\delta &\approx \delta \approx ka(\frac{\tan Ka}{Ka} - 1) \\ \sigma &\approx 4\pi a^2(\frac{\tan Ka}{Ka} - 1)^2\end{aligned}$$

Homework #12: 1. Draw σ vs. V_0 at low energy limit. Confirm that, if we set $\rho = 4.8 \approx Ka$, $\sigma(0) \approx 45\pi a^2$ with two bound states. Discuss physics of the graph.

S-wave resonances: When Ka passes through $n(\pi/2)$, which is just the condition that the well be deep enough for a bound state to develop, then $\tan Ka \to \infty$ and

$$\tan\delta_0 \to \infty$$

that is, δ_0 goes through $n(\pi/2)$ and thus $\sin\delta_0 \approx 1$. It yields that the cross section has maximum and the scattering shows resonances.

$$\sigma_{0,max} = \frac{4\pi}{k^2}, \qquad Ka = n(\pi/2)$$

Transparency: When the beam energy satisfies the transcendental relation

$$\tan Ka = Ka, \qquad \tan\delta_0 \to 0$$

δ_0 becomes zero. It implies that the attractive well scattering reveals transparent. Such resonant transparency is experimentally corroborated in the scattering of low-energy electrons by rare gas atoms. It is called the *Ramsauer Effect.*

Homework #12: 2. Draw σ vs. $\hbar ka$ for a square well potential, $\rho = 4.8$ and confirm a transparency.

2 3-D Square well problem - Bound and scattering states

Consider a particle with a mass of m in a three-dimensional square well potential,

$$V(r) = \begin{cases} \infty & ; \quad -\infty < r < 0 \\ -|V_0| & ; \quad 0 < r < a \\ 0 & ; \quad a < r < \infty \end{cases}$$

The 3-D Schrödinger equation becomes

$$[\frac{\hat{p}^2}{2\mu} + V(r)]\varphi = [\frac{\hat{p}_r^2}{2\mu} + \frac{\hat{\mathbf{L}}^2}{2\mu r^2} + V(r)]\varphi = E\varphi$$

The solution becomes

$$\varphi(r,\theta,\phi) \quad = \quad R(r)Y_{\ell m}(\theta,\phi)$$

Then $R(r)$ satisfies

$$[(\frac{1}{r}\frac{d^2}{dr^2}r) + (k^2(r) - \frac{\ell(\ell+1)}{r^2})]R(r) = 0$$

where

$$K^2(r) \equiv \frac{2m[E - V(r)]}{\hbar^2}$$

Furthermore, if we set $R(r) \equiv \frac{u(r)}{r}$ then, $u(r)$ satisfies

$$[\frac{d^2}{dr^2} + K^2(r) - \frac{\ell(\ell+1)}{r^2}]u(r) \quad = \quad 0$$

For the S-state, it becomes the same problem as that in the one-dimensional problem, as done in the previous section.

In this square well problem, we have $K^2 = \frac{2m[E+V_0]}{\hbar^2}$ = constant. For a constant K, the solutions of $R(r)$ are the regular spherical Bessel function, j_ℓ and irregular spherical Neumann function, n_ℓ. (See Lecture III of last year's lecture.)

In the inner region ($0 < r < a$), there is only one solution that is regular at the origin:

$$Aj_\ell(Kr) \quad \text{(A is a normalization constant.)}$$

In the outer region ($r > a$), $R(r)$ should be that of a free particle.

2.1 Discrete bound state problem, $E < 0$

Let us put again $\kappa^2 = -2mE/\hbar^2$. The only solution bounded at infinity is the exponentially decreasing solution (characteristic of a bound state),

$$Bh_\ell^{(+)}(i\kappa r), \quad h_\ell^{(+)} \equiv n_\ell + ij_\ell$$

which is called the spherical Henkel function, which behaves asymptotically as outgoing and incoming waves (superscript (+)and (-)),

$$h_\ell^{(+)}(\rho \to \infty) \sim \frac{e^{i(\rho - \frac{1}{2}\ell\pi)}}{\rho}, \quad h_\ell^{(-)}(\rho \to \infty) \sim \frac{e^{-i(\rho - \frac{1}{2}\ell\pi)}}{\rho}$$

The continuity matching condition of the function for $r = a$ fixes the ratio B/A. The continuity of the logarithmic derivative yields

$$\frac{1}{h_\ell^{(+)}(i\kappa r)}[\frac{d}{dr}h_\ell^{(+)}(i\kappa r)]|_{r=a} = \frac{1}{j_\ell(Kr)}[\frac{d}{dr}j_\ell(Kr)]|_{r=a}$$

This condition can be fulfilled only for certain discrete values of E. It determines the energy levels of the bound states of the particle. For the S-state, this equation becomes simply

$$Ka\cot Ka = -\kappa a,$$

as obtained in the previous section.

Homework #12: 3. Draw $V_\ell^{eff}(\ell = 0, 1, 2, 3)$ for a square well with $\rho = (2ma^2V_0/\hbar^2)^{1/2} = 4.8$. Obtain the bound states with $\ell = 0, 1, 2, 3$.

2.2 Scattering state problem, $E > 0$

Let us put $k^2 = 2mE/\hbar^2$. We write the outer solution in the form

$$B[\cos\delta_\ell j_\ell(kr) + \sin\delta_\ell n_\ell(kr)]$$

It is indeed easily verified that the asymptotic form of this solution is

$$B\frac{\sin(kr - \frac{1}{2}\ell\pi + \delta_\ell)}{kr}$$

where δ_ℓ is the ℓ-th partial wave phase shift.

The continuity condition of the function at $r = a$ fixes the ratio B/A. Then δ_ℓ is determined by the continuity condition of the logarithmic derivative

$$\begin{aligned}
K\frac{j'_\ell(Ka)}{j_\ell(Ka)} &= k\frac{\cos\delta_\ell j'_\ell(ka) + \sin\delta_\ell n'_\ell(ka)}{\cos\delta_\ell j_\ell(ka) + \sin\delta_\ell n_\ell(ka)} \\
\tan\delta_\ell &= -\frac{j'_\ell(ka) - gj_\ell(ka)}{n'_\ell(ka) - gn_\ell(ka)} \\
g &\equiv \frac{K}{k}\frac{j'_\ell(Ka)}{j_\ell(Ka)}
\end{aligned}$$

The partial scattering amplitude then becomes

$$f_\ell = \frac{1}{k}e^{i\delta_\ell}\sin\delta_\ell = \frac{-1}{k}\frac{j'_\ell(ka) - gj_\ell(ka)}{h'_\ell(ka) - gh_\ell(ka)}$$

where $h_\ell = h_\ell^{(+)}$. The partial cross section becomes

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell = \frac{4\pi}{k^2}(2\ell+1)|\frac{j'_\ell(ka) - gj_\ell(ka)}{h'_\ell(ka) - gh_\ell(ka)}|^2$$

Homework #12: 4. Obtain the partial cross sections with $\ell = 0, 1, 2, 3$ for a square well potential, $\rho = 4.8$ in terms of $\hbar ka$. Answer is in Taylor's book, Fig.11.3.

3 Woods-Saxon potential - Bound and scattering States

Consider a particle with a mass of m in a Woods-Saxon potential,

$$V(r) \quad = \quad -V_0 \frac{1}{1 + \exp[(r - R_0)/a_0]}$$

where R_0 is the radius parameter, and a the diffuseness parameter.

We can solve the bound state problem by using the computer code NEPTUNE and scattering problem by VENUS.

Homework #13: 1. Draw $V_\ell^{eff}(\ell = 0, 1, 2, 3)$ for a Woods-Saxon potential, $V_0 = 425$ MeV, $R_0 = 1.5$ fm and $a_0 = 0.5$ fm. Obtain the binding energies and partial cross sections with $\ell = 0, 1, 2, 3$.

4 Jost function

We now are back to the radial Schrödinger equation

$$[\frac{d^2}{dr^2} + U(r) - \frac{\ell(\ell+1)}{r^2} + k^2]\chi_{\ell,k}(r) = 0$$

Remember that we deal with $\chi_{\ell,k}(r)$, not $R(r) = \chi_{\ell,k}(r)/r$. In the scattering state,

$$\chi_{\ell,k}(r \to \infty) \to e^{i\delta_\ell} \sin[kr - \frac{1}{2}\ell\pi + \delta_\ell(k)]$$

At large r, $\chi_{\ell,k}(r)$ is proportional to the free radial function

$$j_\ell(kr) \to \sin(kr - \frac{1}{2}\ell\pi)$$

Another boundary condition is that at $r = 0$, $\chi_{\ell,k}(r) = 0$. We call such a solution the regular solution $\phi_{\ell,k}(r)$. We wish to discuss a solution that is defined by two boundary conditions with a single function. For this reason, we define the **regular solution**, $\phi_{\ell,k}(r)$, as the solution that behaves exactly like $j_\ell(kr)$ as $r \to 0$,

$$\phi_{\ell,k}(r \to 0) \to j_\ell(kr)$$

4.1 Behavior of $\phi_{\ell,k}$ for large r and definition of the Jost function.

As $r \to \infty$, $\phi_{\ell,k}$ must approach some combination of solutions of the free radial equation, $ah^- + bh^+$, say. ($h_\ell^\pm = n_\ell \pm ij_\ell$.) Remembering that $\phi_{\ell,k}$ is real and inserting a factor $i/2$ for convenience, we can write this as

$$\phi_{\ell,k}(r \to \infty) \longrightarrow \frac{i}{2}[\mathcal{F}_\ell(k)h_\ell^-(kr) - \mathcal{F}_\ell^*(k)h_\ell^+(kr)]$$

where the coefficient $\mathcal{F}_\ell$ is called the *Jost function*.

4.2 Properties of the Jost function

The regular solution $\phi_{\ell,k}$ is proportional to the normalized function $\chi_{\ell,k}$ whose asymptotic form is

$$\chi_{\ell,k}(r \to \infty) \longrightarrow \frac{i}{2}[h_\ell^-(kr) - S_\ell(k)h_\ell^+(kr)]$$

Comparing these two forms we see that

$$S_\ell = \frac{\mathcal{F}_\ell^*(k)}{\mathcal{F}_\ell(k)}$$
$$\phi_{\ell,k}(r) = \mathcal{F}_\ell(k)\chi_{\ell,k}(r)$$

The Jost function is just the ratio of the two solutions
$\phi_{\ell,k}(r)$ and $\chi_{\ell,k}(r)$.
S_ℓ has modulus unity (i.e., unitary).
Since $S_\ell = \exp(2i\delta_\ell)$,

$$\mathcal{F}_\ell(k) = |\mathcal{F}_\ell(k)| \exp(-i\delta_\ell(k))$$

4.3 $\mathcal{F}_\ell(k)$ in terms of $\phi_{\ell,k}(r)$

The Lippmann-Schwinger equation for $\chi_{\ell,k}(r)$ is

$$\chi_{\ell,k}(r) = j_\ell(r) + \int_0^\infty dr' G_{\ell,k}(r,r') U(r') \chi_{\ell,k}(r')$$

For $\phi_{\ell,k}(r)$, the integral equation becomes

$$\begin{aligned}
\phi_{\ell,k}(r) &= j_\ell(r) + \lambda \int_0^r dr' g_{\ell,k}(r,r') U(r') \phi_{\ell,k}(r') \\
g_{\ell,k}(r,r') &= \frac{1}{k}[j_\ell(kr) n_\ell(kr') - n_\ell(kr) j_\ell(kr')] \\
&= \frac{i}{2k}[h_\ell^-(kr) h_\ell^+(kr') - h_\ell^+(kr) h_\ell^-(kr')]
\end{aligned}$$

where λ guarantees smallness of $U(r)$.

As $r \to \infty$,

$$\begin{aligned}
\phi_{\ell,k}(r) \quad \to \quad & \frac{i}{2}\{[1 + \frac{\lambda}{k} \int_0^\infty dr' h_\ell^+(kr') U(r') \phi_{\ell,k}(r')] h_\ell^-(kr) \\
& - [.....]^* h_\ell^+(kr)\}
\end{aligned}$$

Comparing this with the equation where the Jost function is defined above, we have

$$\mathcal{F}_\ell(k) = 1 + \frac{\lambda}{k} \int_0^\infty dr h_\ell^+(kr) U(r) \phi_{\ell,k}(r)$$

4.4 Schwarz reflection principle

The principle says that
"If $f(z)$ is analytic in a region $\mathcal{R}$ that includes a segment of the real axis, and $f(z)$ is real on this segment, then $f(z)$ can be continued onto the region $\mathcal{R}*$ and satisfies $f(z) = [f(z^*)]^*$ for all z in $\mathcal{R}$ and $\mathcal{R}*$."

Making $k \to ik$, we have

$$\mathcal{F}_\ell(k) = [\mathcal{F}_\ell(-k^*)]^*$$

In particular, for k pure imaginary, $\mathcal{F}_\ell(k)$ is real.

5 Analytic properties of the Jost function and S matrix

5.1 Analytic functions of a complex variable

"A function $f(z)$ is said to be *analytic* (or holomorphic, or regular) in the complex variable z, on some region $\mathcal{R}$."

Example: $\sin z$ is analytic everywhere.
$1/z$ is analytic except at $z = 0$
where it has a pole.

Cauchy's theorem leads to further results:

(1) An analytic function is actually infinitely differentiable.
(2) It can be expanded as a power series about any point in $\mathcal{R}$.
(3) If $f(z)$ is analytic except at a number of poles, then the integral $\oint dz f(z)$ around any closed path is $2\pi i$ times the sum of residues at those poles inside the contour.

5.2 Analytic properties of the regular solution

Consider again the radial Schrödinger equation

$$[\frac{d^2}{dr^2} + U(r) - \frac{\ell(\ell+1)}{r^2} + k^2]\chi_{\ell,k}(r) \quad = \quad 0$$

We now suppose k to be an arbitrary complex number. In the complex plane of k only those points on the positive real axis ($p \geq 0$) are relevant to the actual physical scattering problem; for this region we refer to **the positive real axis as the "physical region"**.

We wrote the regular solution as

$$\begin{aligned}
\phi_{\ell,k}(r) &= j_\ell(r) + \int_0^r dr' g_{\ell,k}(r,r')U(r')\phi_{\ell,k}(r') \\
g_{\ell,k}(r,r') &= \frac{1}{k}[j_\ell(kr)n_\ell(kr') - n_\ell(kr)j_\ell(kr')]
\end{aligned}$$

The free solution $j_\ell(r)$ and Green's function $g_{\ell,k}(r,r')$ are well defined and, in fact, analytic for all k. The same is true of the regular function $\phi_{\ell,k}(r)$. (See Taylor's book, Section 12-b.)

5.3 Analytic properties of the Jost function

The Jost function is defined as

$$\mathcal{F}_\ell(k) = 1 + \frac{1}{k}\int_0^\infty dr h_\ell^+(kr)U(r)\phi_{\ell,k}(r)$$

When k becomes complex, we can prove (See Taylor's Problem 12.1.) that in general $\phi_{\ell,k}(r)$ grows exponentially like

$$\begin{aligned}
\phi_{\ell,k}(r \to \infty) &\longrightarrow e^{|Imkr|} \\
h_{\ell,k}^+(r \to \infty) &\longrightarrow e^{i(kr - 1/2\ell\pi)} \propto e^{-Imkr}
\end{aligned}$$

Thus $h_{\ell,k}^+(r)$ grows exponentially for $\Im k < 0$, but decreases exponentially for $\Im k > 0$. In the lower half plane of k space, the integral will in general diverge exponentially, while in the upper the growth of $\phi_{\ell,k}$ is canceled by the decrease of h^+ and the integral converges. We summarize that the Jost function is

$$\begin{aligned} \text{physical region} &= \{k \text{ real} \geq 0\} \\ \mathcal{F}_\ell(k) &\text{ analytic in}\{\Im k > 0\} \end{aligned}$$

We now summarize the Jost function;

$$\begin{aligned} \mathcal{F}_\ell(k) &= \frac{\phi_{\ell,k}(r)}{\chi_{\ell,k}(r)}, \\ &= |\mathcal{F}_\ell(k)| \exp(-i\delta_\ell(k)), \\ &= 1 + \frac{\lambda}{k} \int_0^\infty dr h_\ell^+(kr) U(r) \phi_{\ell,k}(r), \\ &= [\mathcal{F}_\ell(-k^*)]^*, \\ &\quad \text{analytic in}\{\Im k > 0\} \end{aligned}$$

5.4 Analytic properties of the S_ℓ matrix

The S_ℓ matrix, which for physical $k \geq 0$ was given by

$$S_\ell = \frac{\mathcal{F}_\ell^*(k)}{\mathcal{F}_\ell(k)} \quad [k \geq 0]$$

In this form of S_ℓ is certainly not analytic since $\mathcal{F}_\ell^*(k)$ is not. However, remembering that k is real,

$$S_\ell = \frac{\mathcal{F}_\ell^*(k^*)}{\mathcal{F}_\ell(k)} = \frac{\mathcal{F}_\ell(-k)}{\mathcal{F}_\ell(k)}$$

In either of these equivalent forms of S_ℓ is the quotient of two analytic functions. Unfortunately, the denominator is analytic for $\Im k > 0$, while the numerator is analytic for $\Im k < 0$. Thus we have failed to establish any region of analyticity of S_ℓ at all.

6 Bound states and poles of the S_ℓ matrix

We start with the asymptotic behavior of the regular function

$$\phi_{\ell,k}(r \to \infty) \longrightarrow \frac{i}{2}[\mathcal{F}_\ell(k)h_\ell^-(kr) - \mathcal{F}_\ell(-k)h_\ell^+(kr)]$$

This relation does not always hold once k moves up from the real axis, since $\mathcal{F}_\ell(-k)$ does not necessarily continue there. However, let us suppose for a moment that the potential is such that it does, and suppose that at some point $\bar{k}(\Im\bar{k} > 0)$ the Jost function vanishes, $\mathcal{F}_\ell(\bar{k}) = 0$. In this case,

$$\phi_{\ell,\bar{k}}(r \to \infty) \longrightarrow \frac{-i}{2}\mathcal{F}_\ell(-\bar{k})h_\ell^+(\bar{k}r)$$

Now as $r \to \infty$,

$$h_\ell^\pm(kr) \to e^{\pm i(kr - \ell\pi/2)}$$

$h_{\ell,k}^+(r)$ decreases exponentially for $\Im k > 0$ while $h_{\ell,k}^-(r)$ increases exponentially. It follows that $\phi_{\ell,\bar{k}}$ contains both increasing and decreasing components. But at the point $\bar{k}$, where $\mathcal{F}_\ell(\bar{k}) = 0$ vanishes and the above equation holds, ϕ is purely decreasing. Since $\phi_{\ell,\bar{k}}(r)$ vanishes at $r = 0$ and decreases exponentially as $r \to \infty$, it is a normalizable solution of the radial Schrödinger equation with $k = \bar{k}$ and angular momentum ℓ. That is, the Hamiltonian has a proper eigenstate of energy $\hbar^2\bar{k}^2/2m$ and angular momentum ℓ. Since all eigenvalues of H are real, $\bar{k}$ must be in fact be pure imaginary, $\bar{k} = i\alpha(\alpha > 0$ and the energy of the bound state is $-\alpha^2/2m$.

Conversely, if the Hamiltonian has a bound state with energy $-\hbar^2\alpha^2/2m$ and angular momentum ℓ, then at the point $k = i\alpha$ the solution $\phi_{\ell,\bar{k}}(r)$ must be exponentially decreasing, and according to the first equation of this section, $\mathcal{F}_\ell(i\alpha)$ must be zero.

Provided $\mathcal{F}_\ell(-k)$ is also analytic at $k = \bar{k} = i\alpha$ we can equivalently say that the bound states correspond to poles of $S_\ell(k) = \mathcal{F}_\ell(-k)/\mathcal{F}_\ell(k)$. Indeed we can understand this result directly if we recall that $S_\ell(k)$ is simply the ratio of outgoing to incoming wave in ϕ. When $\Im k > 0$ outgoing waves decreases as $r \to \infty$, while incoming waves increase. Since at a bound state ϕ is purely decreasing, the ratio $S_\ell(k)$ has to be infinite.

7 Levinson's theorem

Theorem: For any spherical potential, the phase shift $\delta_\ell(k)$ satisfies

$$\delta_\ell(0) - \delta_\ell(\infty) = n_\ell \pi$$

where n_ℓ denotes the number of bound states of angular momentum ℓ.

The exceptional case is that the s-wave Jost function vanishes at threshold, $\mathcal{F}_0(0) = 0$. In this cae

$$\delta_0(0) - \delta_0(\infty) = (n_0 + \frac{1}{2})\pi$$

Proof: We consider the integral

$$I = \oint dk \frac{1}{\mathcal{F}_\ell(k)} \frac{d\mathcal{F}_\ell(k)}{dk} = \oint d \ln \mathcal{F}_\ell(k) = \int_{-\infty}^{\infty} d \ln \mathcal{F}_\ell(k)$$

The integrand $\frac{1}{\mathcal{F}_\ell} \frac{d\mathcal{F}_\ell}{dk}$ is analytic on and inside the contour except that at each simple zero of $\mathcal{F}_\ell$ which has a pole with residue one. By the Cauchy's theorem,

$$I = 2\pi i n_\ell$$

The contribution of the large semicircle is zero. Now, on the positive real axis

$$\mathcal{F}_\ell(k) = |\mathcal{F}_\ell(k)| e^{-i\delta_\ell(k)} \qquad [k \geq 0]$$

and, hence

$$\ln \mathcal{F}_\ell(k) = \ln |\mathcal{F}_\ell(k)| - i\delta_\ell(k)$$

On the negative real axis we use the relation $\mathcal{F}_\ell(-k) = \mathcal{F}_\ell(k)^*$ to give

$$\ln \mathcal{F}_\ell(-k) = \ln |\mathcal{F}_\ell(k)| + i\delta_\ell(k) \quad [k > 0]$$

Inserting these results into the integration I above, we find that the contributions of the real parts from the positive and negative axes cancel an that

$$\begin{aligned} I &= -2i \int_0^\infty d\delta_\ell(k) \\ &= 2i[\delta_\ell(0) - \delta_\ell(\infty)] \end{aligned}$$

Comparing two I's gives the proof.

For the exceptional case, consult with Taylor's Section 12-g.

Homework #14: 1. Similar to Homework #3, obtain the partial cross sections with $\ell = 3$ for a square well potential, $\rho = 5.2,\ 5.5,\ 5.7,\ 5.8$ in terms of $\hbar ka$.
Answer is in Taylor's book, Fig.13.7.
2. Count # of bound states for each potential.
3. Obtain the partial cross sections with $\ell = 1$ for a Woods-Saxon potential, $V_0 = 29.84$ MeV, $V_{SO} = -8.24$ MeV, $R_0 = R_{SO} = 2.95$ fm (not reduced) and $a_0 = a_{SO} = 0.52$ fm in the ^{7}Be + p system at energies between 0.1 MeV and 2.0 MeV.

8 Resonances and poles of the S_ℓ matrix

Suppose that the Jost function has a zero (hence S_ℓ a pole) in the lower half plane close to the real axis, and explore in physically observable consequences. It is essential that the potential be such as to allow continuation into $\{\Im k < 0\}$. We shall assume that this is the case.

Since $\mathcal{F}_\ell(-k)$ is always analytic in $\{\Im k < 0\}$ and $\mathcal{F}_\ell(\pm k)$ can not both vanish at the same point, $\mathcal{F}_\ell(k)$ vanishes at some point $\bar{k}$ in $\{\Im k < 0\}$ *if and only if* $S_\ell(k) = \mathcal{F}_\ell(-k)/\mathcal{F}_\ell(k)$ has a pole. Thus, there is a complete equivalence between zeros of $\mathcal{F}_\ell(k)$ and poles of $S_\ell(k)$ in $\{\Im k < 0\}$.

Assume that $\mathcal{F}_\ell(k)$ has a zero at some point

$$\bar{k} = k_R - ik_I[k_I > 0]$$

and further that this zero is simple. Thus there is some neighborhood of k in which we can approximate $\mathcal{F}_\ell(k)$ as

$$\mathcal{F}_\ell(k) \approx (\frac{d\mathcal{F}_\ell(k)}{dk})_{\bar{k}}(k - \bar{k})$$

Recall that for physical k the phase shift is minus the phase of $\mathcal{F}_\ell(k)$. Thus we have

$$\begin{aligned}
\delta(k) &\approx -\arg(\frac{d\mathcal{F}_\ell(k)}{dk})_{\bar{k}} - \arg(k - \bar{k}) \\
&\equiv \delta_{bg} + \delta_{res} \\
\delta_{res}(k) &= -\arg(k - \bar{k})
\end{aligned}$$

The quantity δ_{bg} is called the *background phase shift* and is just minus the phase of $(\frac{d\mathcal{F}_\ell(k)}{dk})_{\bar{k}}$. The quantity δ_{res} is called the *resonant part of the phase shift* and is the angle shown in Fig. 13.2.

It is clear from the figure that as k increases past the location of the zero, the resonant part of the phase shift $\delta_{res}(k)$ increases from 0 to π. Also, the closer the zero is to the real axis, the more suddenly this increases occurs. (For example, δ_{res} increase from $\pi/4$ to $3\pi/4$ in the interval of width $2k_I$ between $k = k_R \pm k_I$.) Thus near a zero of $\mathcal{F}_\ell(k)$ that is close to the real axis, the complete phase shift $\delta = \delta_{bg} + \delta_{res}$ increases suddenly from value δ_{bg} to $\delta_{bg} + \pi$.

The behavior of the partial cross section $\sigma_\ell(k)$,

$$\sigma_\ell(k) = 4\pi\frac{2\ell + 1}{k^2}\sin^2\delta_\ell(k)$$

near a resonance depends on the value of the background δ_{bg}. Four different possibilities are shown in Fig. 13.3.

Type	δ_{bg}	$\delta(k)$	Characteristics
(a)	0	0 to π	a sharp peak at $\pi/2$.
		(sudden change)	Breit-Wigner resonance
(c)	$\pi/2$	$\pi/2$ to $3\pi/2$	a sharp minimum thru π.
(b,d)			Intermediate cases.

8.1 Breit-Wigner formula

Consider $\mathcal{F}_\ell(E)$ instead of $\mathcal{F}_\ell(k)$. Since the mapping from k to E is two-to-one, $\mathcal{F}_\ell(E)$ is a function on a *two-sheeted Riemann surface*. See Fig. 13.4. The first sheet or "physical sheet" of E corresponds to the upper half plane $\{\Im k > 0\}$, the second sheet to the lower half plane $\{\Im k < 0\}$.

If the Jost function as a function of E, then resonance zero at $\bar{k}$ becomes a zero on the second sheet, close to the physical region, at

$$\bar{E} = \frac{\hbar^2 k^2}{2m} = E_R - \frac{i\Gamma}{2}$$

The notation of $\Gamma/2$ for the imaginary part of $\bar{E}$ is conventional. Close to the resonance we write $\mathcal{F}_\ell(E) = (d\mathcal{F}_\ell(E)/dE)_{\bar{E}}(E - \bar{E})$ and, as before, we find that for real E close to E_R,

$$\delta_\ell(E) \approx \delta_{bg} + \delta_{res}(E) \quad [E \text{ real, close to } E_R].$$

The resonant part of the phase shift $\delta_{res}(E)$ is the angle shown in Fig. 13.4 and we have

$$\sin\delta_{res}(E) = \frac{\Gamma/2}{[(E - E_R)^2 + (\Gamma/2)^2]^{1/2}}$$

If $\delta_{bg} \approx 0$, the partial cross section yields

$$\sigma_\ell(E) \propto \sin^2\delta_{res}(E) = \frac{(\Gamma/2)^2}{[(E - E_R)^2 + (\Gamma/2)^2]}$$

This is the famous *Breit-Wigner formula* which gives a peak at E_R and has width Γ.

9 Bound states and resonances

9.1 Low energy behavior of the Jost function

Assume that the potential is exponentially bounded so that $\mathcal{F}_\ell(k)$ is actually analytic near $k = 0$. We insert into the integral

$$\begin{aligned}\mathcal{F}_\ell(k) &= 1 + \frac{1}{k}\int \hat{h}^+ U\phi \\ &= 1 + \frac{1}{k}\int \hat{n}^+ U\phi + i\frac{1}{k}\int \hat{j} U\phi\end{aligned}$$

the expansions of $\hat{n}, \hat{j}$ and ϕ in powers of k. (Recall that $\hat{n}(x) = xn(x)$, etc.)

Function	Asymptotic form	low energy behavior
$\hat{j}$	$\sim \frac{(kr)^\ell+1}{(2\ell+1)!!}[1 + O(x^2)]$	$\sim k^{\ell+1}[1 + O(x^2)]$
$\hat{n}$	$\sim \frac{(2\ell-1)!!}{(kr)^\ell}[1 + O(x^2)]$	$\sim k^{-\ell}[1 + O(x^2)]$
ϕ	$\sim \frac{(kr)^\ell+1}{(2\ell+1)!!}[1 + O(x^2)]$	$\sim k^{\ell+1}[1 + O(x^2)]$

Thus $\mathcal{F}_\ell(k)$ has the form:

$$\mathcal{F}_\ell(k) = 1 + [\alpha_\ell + \beta_\ell k^2 + O(k^4)] + i\gamma_\ell k^{2\ell+1} + O(k^{2\ell+3})]$$

The Jost function $\mathcal{F}_\ell(k)$ vanishes at $k = 0$, if it happens that α_ℓ has the value -1. When this happens

$$\mathcal{F}_\ell(k) = [\beta_\ell k^2 + O(k^4)] + i[\gamma_\ell k^{2\ell+1} + O(k^{2\ell+3})]$$

For the $s-$wave case, the leading term is

$$\mathcal{F}_{\ell=0}(k) = i\gamma_0 k + O(k^2)$$

while for any $\ell > 0$ it comes from the first bracket

$$\mathcal{F}_\ell(k) = \beta_\ell k^2 + O(k^3 \text{ or } k^4) \qquad [\ell > 0]$$

Thus, if the Jost function has a zero at $k = 0$, then for $\ell = 0$ this zero is simple, while for $\ell > 0$ it is double.

9.2 Virtual state (Zero of the $s-$wave the Jost function)

We introduce the variable coupling parameter λ and Hamiltonian $H = H_0 + \lambda V$. Generally, the Jost function $\mathcal{F}_\ell(\lambda, k)$ is analytic function of both λ and k, for all λ and all k except for the usual singularities in $\{\Im k < 0\}$. We then make a double power expansion series of $\mathcal{F}_\ell(\lambda, k)$ in λ and k about the point $\lambda = \lambda_0$, and $k = 0$,

$$\mathcal{F}_\ell(\lambda, k) = \sum_{m,n} \alpha_{m,n} k^m (\lambda - \lambda_0)^n$$

For the case $\ell = 0$, the zero at threshold is simple, the lowest terms of the double power series become

$$\mathcal{F}_\ell(\lambda, k) = i\xi k + \eta(\lambda - \lambda_0) + ...$$

(with ξ and η are real). Obviously when $\lambda = \lambda_0$ this has the simple zero at $k = 0$, while for λ close to λ_0 the same zero is found to be found at

$$\bar{k} \approx -i\frac{\eta}{\xi}(\lambda - \lambda_0) \qquad [\ell = 0]$$

That is, as λ moves past λ_0 (with real values) the zero moves linearly down to the imaginary axis as shown in Fig. 13.5(a). The corresponding motion of the zero on the Riemann surface of E is shown in Fig.13.5(b).

In Fig. 13.5(a), the zero of the s-wave Jost function is starting in $\{\Im k > 0\}$ as a bound state. As the potential weakens the bound state moves down the imaginary axis and becomes progressively less well bound until, when $\lambda = \lambda_0$, it becomes a zero-energy resonance. As we continue to weaken the potential the zero moves on down the imaginary axis. It clearly does not remain close to the real axis and, hence, does not become a resonance of the type we discussed in Sec. II-8.

The zero of the s-wave Jost function on the negative imaginary axis is referred to as a *virtual state*. Obviously a virtual state is not a proper bound state. A virtual state close to the origin implies that $\mathcal{F}_0(0)$ is small and, hence, the scattering length is large. Thus, a virtual state close to threshold causes a large cross section at low energy.

9.3 Resonances with $\ell > 0$

We know that the zero at threshold is a double zero, and the double power series for $\mathcal{F}_\ell(\lambda, k)$ has the form

$$\mathcal{F}_\ell(\lambda, k) = \xi k^2 + \eta(\lambda - \lambda_0) + ... \quad [\ell > 0]$$

When λ is close to λ_0, this has two zeros at

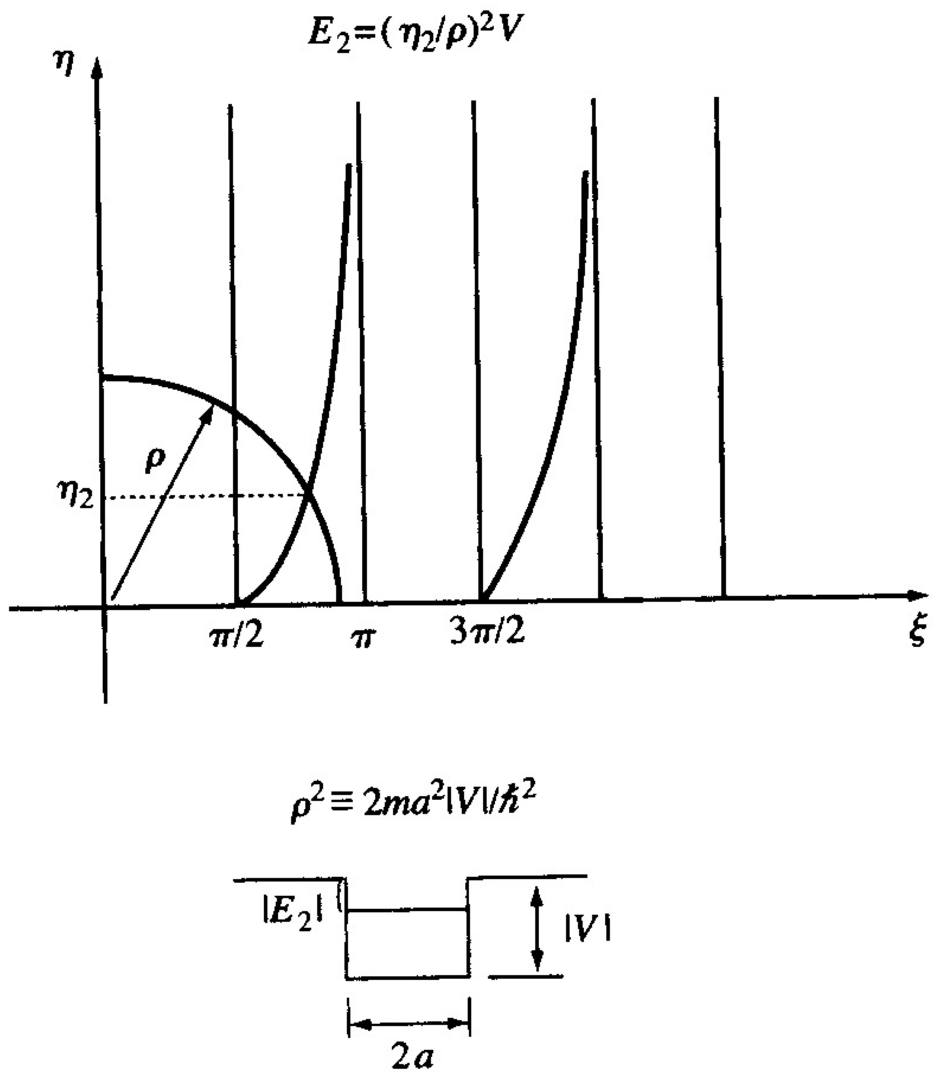
$$\bar{k} \approx \pm i(\frac{\eta}{\xi})^{1/2}(\lambda - \lambda_0)^{1/2} \quad [\ell > 0]$$

As λ moves through λ_0, these two zeros coalesce at the origin and part company as shown in Fig. 13.6(a).

When the potential is slightly more attractive than at λ_0 the two zeros lie on the imaginary axis, one above the origin representing a bound state, and the other below. As $\lambda \to \lambda_0$, the zeros move inwards until, when $\lambda = \lambda_0$, both are at the origin and there is a zero-energy bound state. As λ moves past λ_0 the zeros leave the origin tangentially to the real axis. They cannot move into the upper half plane or onto the real axis, and they thus move into the lower half plane as shown. In particular, the zero on the right becomes a resonance and continues as such until it finally moves too far away from the axis to be observable.

In conclusion, we remark that for certain systems it is possible that all resonances are "would-be bound state" of the type just discussed. In this case bound states and resonances could be regarded as essentially the same thing; both would be zeros of $\mathcal{F}$ (or poles of S), the only distinction being that the bound states happen to lie in $\{\Im k > 0\}$, the resonances in $\{\Im k < 0\}$. A "democratic" arrangement of this type has been much discussed as a natural scheme for the elementary particles. However, appealing as this scheme undoubtedly is, we should perhaps close by repeating that there certainly are systems for which the situation is more complicated, for which some resonances do not correspond to poles of S, and for which some poles of S do not correspond to resonances.

4. Resonances–Figures



Liboff Figure 8.3

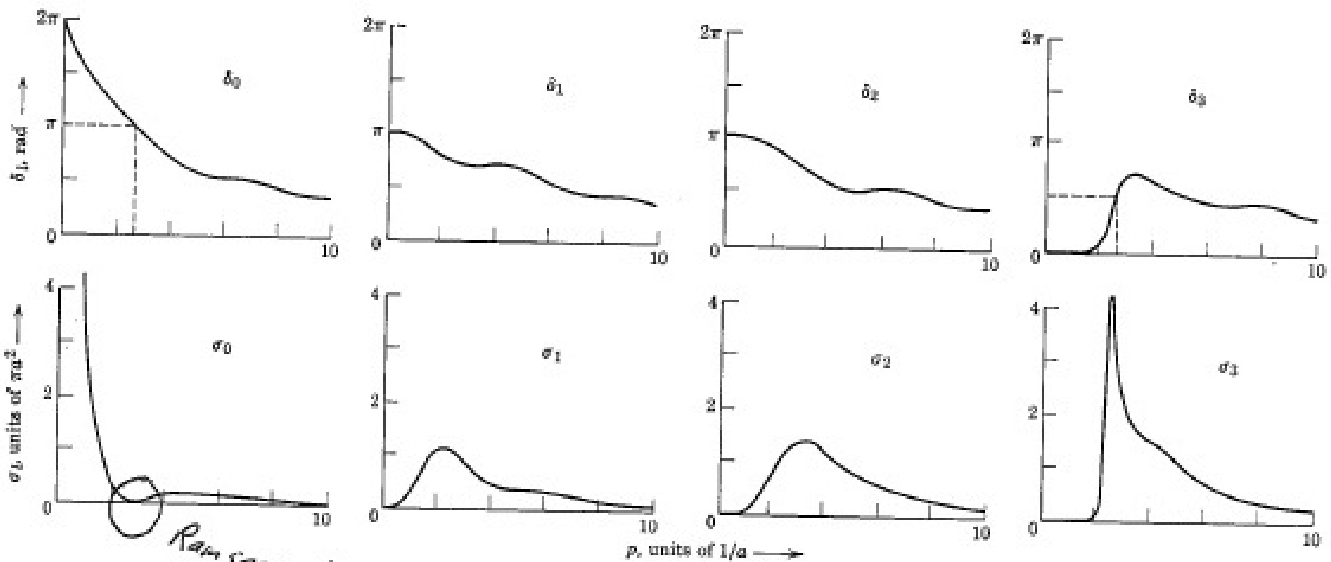
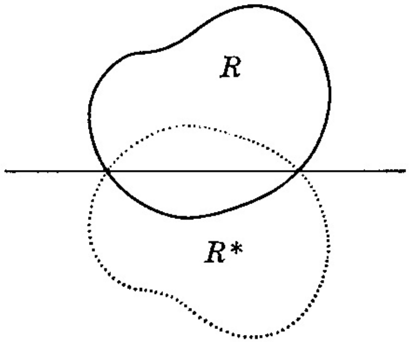


FIGURE 11.3. Phase shifts $\delta_l(p)$ and partial cross sections $\sigma_l(p)$ for a square well of depth V_0 given by $(2ma^2V_0)^{1/2} = 4.8$.

Taylor Fig. 11.3



Schwarz reflection principle

FIGURE 12.2. When $f(z)$ is analytic on R, then $g(z) = [f(z^*)]^*$ is analytic on R^*.

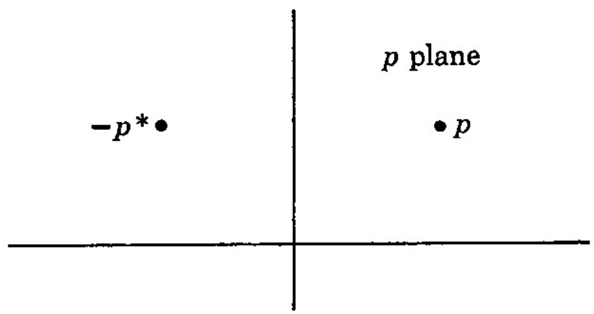


FIGURE 12.3. The Jost function is analytic for $\operatorname{Im} p > 0$ and real on the imaginary axis. By the Schwartz principle $\mathscr{f}(p) = [\mathscr{f}(-p^*)]^*$.

Taylor 12.2 & 12.3

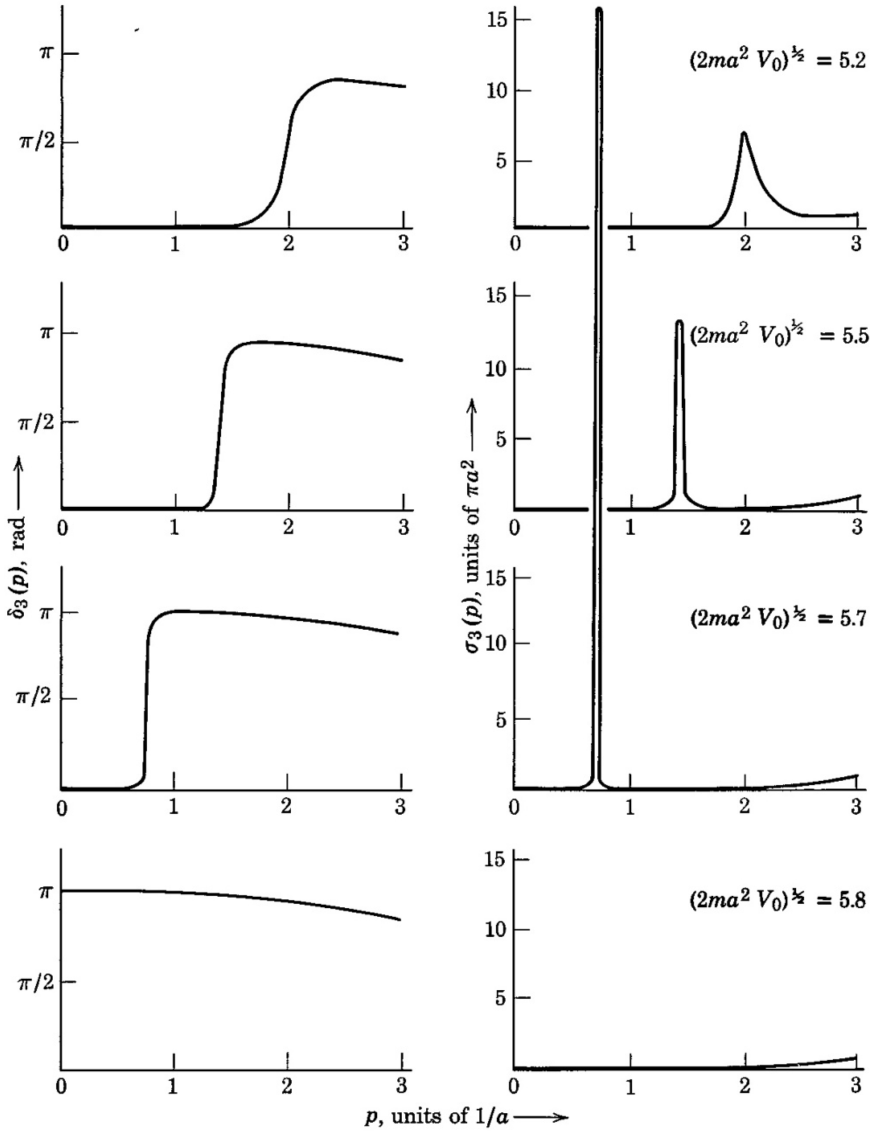


FIGURE 13.7. The $l = 3$ phase shifts and cross sections for four successively deeper square wells. The top three wells are too shallow to support an $l = 3$ bound state—the fourth just can.

Taylor Fig. 13.7

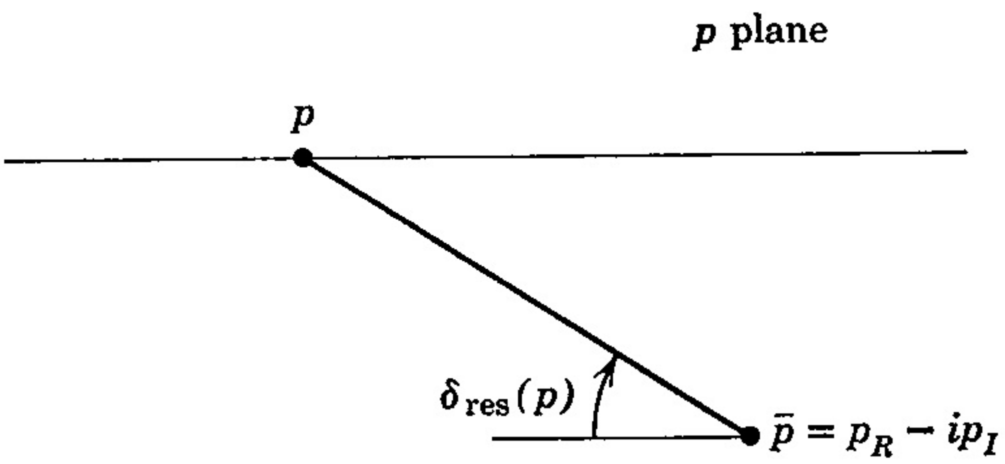


FIGURE 13.2 Resonant part $\delta_{res}(p)$ of phase shift.

Taylor Fig. 13.2

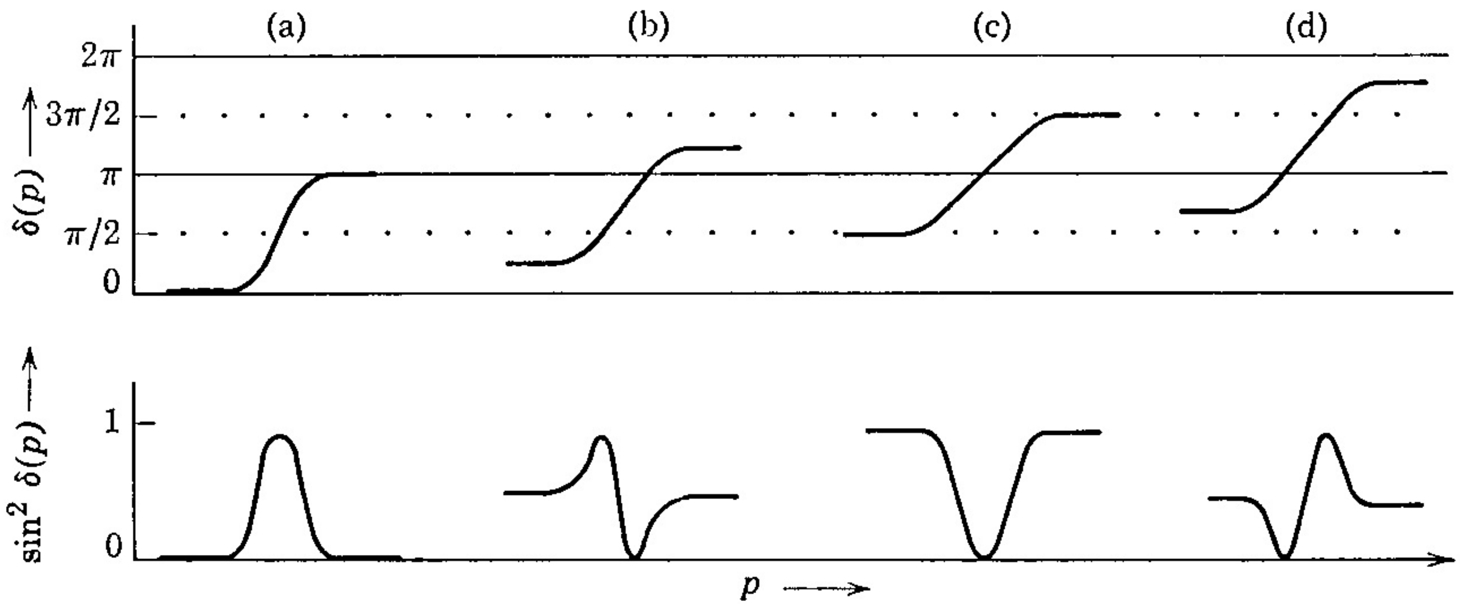


FIGURE 13.3. **Four possible resonances. The $\delta(p)$ plots show the resonant phase shifts for $\delta_{bg} = 0, \pi/4, \pi/2,$ and $3\pi/4$. The $\sin^2 \delta(p)$ plots show the corresponding behavior of the partial cross section [apart from a factor $4\pi(2l + 1)/p^2$].**

Taylor Fig. 13.3

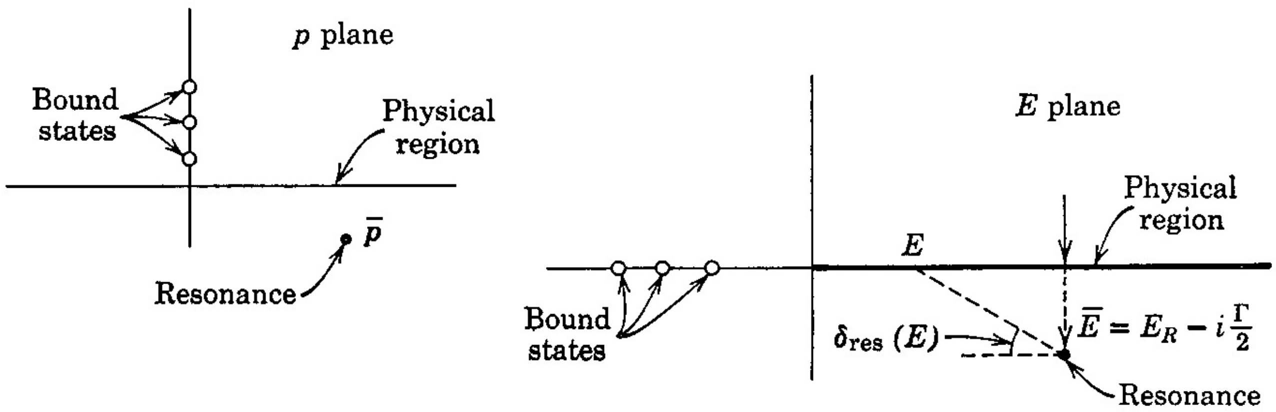


FIGURE 13.4. Planes of the complex variables p and $E = p^2/2m$.

Taylor Fig. 13.4

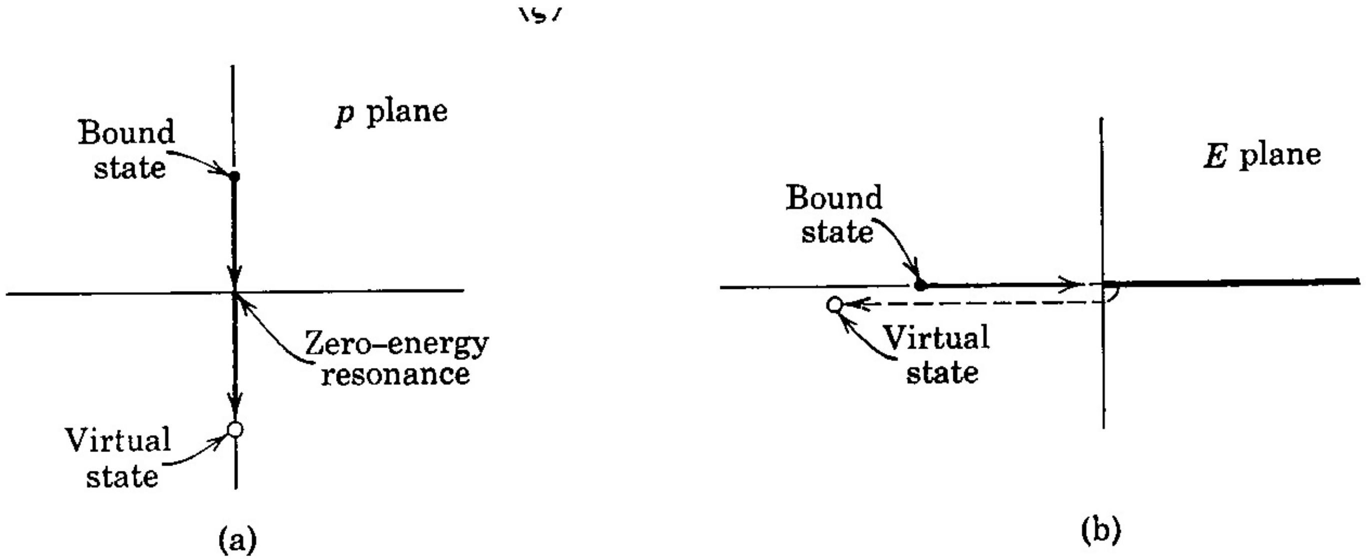


FIGURE 13.5. **(a) Transition of an *s*-wave bound state into a "virtual state." (b) On the Riemann surface of *E* the bound state is on the physical sheet, the virtual state on the second sheet.**

Taylor Fig. 13.5

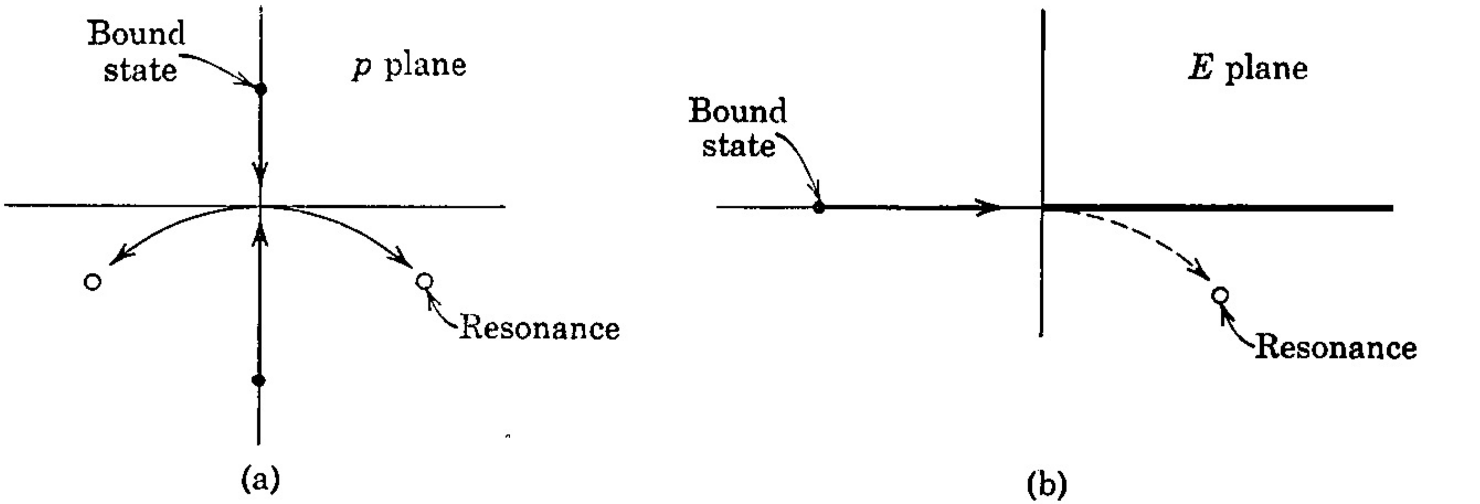


FIGURE 13.6. (a) Transition of a bound state with $l > 0$ into a resonance. (b) Corresponding motion in the E plane (showing only the physically relevant zeros).

Taylor Fig. 13.6