2 Review of Scattering Theory

As we have seen in the introduction, the tools of scattering theory—phase shifts, bound states, and the Born approximation—are central to our calculational techniques. In this chapter, we develop these tools and derive the key results we will need. We focus particularly on the use of the analytic structure of the scattering data to efficiently compute the Green and Jost functions.

For those readers who are more interested in field theory applications, much of the technical discussion in this chapter can be skipped on a first reading. More comprehensive discussion of these subjects can be found in standard references on scattering theory, such as [1, 2].

2.1 Scattering Theory in Arbitrary Dimension

Our ultimate goal is to apply scattering theory to calculations in quantum field theory. Because we will cut off the divergences of quantum field theory using dimensional regularization, it will be important to us to be able to carry out scattering theory calculations in arbitrary dimensions with generalized spherical symmetry. Our starting point is the time-independent Schrödinger equation for the wavefunction with energy $\omega = \pm\sqrt{k^2+m^2}$ in partial wave ℓ of a radially symmetric potential in n space dimensions,

$$-\psi'' + \frac{1}{r^2}\left(\alpha - \frac{1}{2}\right)\left(\alpha + \frac{1}{2}\right)\psi + \sigma(r)\psi - k^2\psi = 0\,, \tag{2.1}$$

where

$$\alpha = \ell - 1 + \frac{n}{2}.$$

To set up a regular scattering problem, we assume that the background potential σ is sufficiently localized, so that

$$\int_0^\infty r\sigma(r)dr < \infty\,. \tag{2.2}$$

Asymptotically, the scattered particles become free, and their behavior as $r \to \infty$ should be compared to the free outgoing spherical wave[1]

[1] Whenever a fractional power of k appears it should be considered as the limit $\mathsf{Im}\, k \searrow 0$.

Graham, N., et al.: *Review of Scattering Theory*. Lect. Notes Phys. **777**, 15–32 (2009)
DOI 10.1007/978-3-642-00139-0_2

$$w_\ell(kr) = (-1)^{\alpha+1}\sqrt{\frac{\pi}{2}kr}\,\left[J_\alpha(kr) + iY_\alpha(kr)\right] , \tag{2.3}$$

where J_α and Y_α are the Bessel functions of first and second kind, respectively [3]. Next we define various solutions to Eq. (2.1) that only differ in the boundary conditions that they obey:

- The *Jost solution*, $f_\ell(k, r)$. It behaves like an outgoing wave at $r \to \infty$, with
$$\lim_{r\to\infty} \frac{f_\ell(k,r)}{w_\ell(kr)} = 1 . \tag{2.4}$$
For $k \neq 0$ the two solutions $f_\ell(\pm k, r)$ are linearly independent because their Wronskian is non-zero.
- The *regular solution*, $\phi_\ell(k, r)$. It is defined by its k-independent behavior near the origin[2]
$$\lim_{r\to 0} \frac{\Gamma(\alpha+1)}{\sqrt{\pi}} \left(\frac{r}{2}\right)^{-(\alpha+\frac{1}{2})} \phi_\ell(k,r) = 1 , \tag{2.5}$$
which determines this solution uniquely. The k-independence implies that $\phi_\ell(k, r)$ is an even function of k (since the Schrödinger equation is) and holomorphic in k for all radii r. By completeness, ϕ_ℓ can be represented as a linear combination of the two Jost solutions,
$$\phi_\ell(k,r) = \frac{i}{2}\left[k^{-\alpha-\frac{1}{2}} F_\ell(k) f_\ell(-k,r) + (-k)^{-\alpha-\frac{1}{2}} F_\ell(-k) f_\ell(k,r)\right] . \tag{2.6}$$
When evaluating fractional exponents in Eq. (2.6), k and $-k$ must be connected by paths in the upper-half k-plane (see property (1) below) [2]. The coefficient function is called the *Jost function*; it can be computed from the Wronskian of ϕ_ℓ and f_ℓ. Alternatively, it can also be read off from the asymptotic behavior of the Jost solution $f_\ell(k, r)$ near the origin,
$$F_\ell(k) = \lim_{r\to 0} \frac{f_\ell(k,r)}{w_\ell(kr)} . \tag{2.7}$$
- The *physical scattering solution*, $\psi_\ell(k, r)$. It is also regular at the origin and thus proportional to $\phi_\ell(k, r)$, but differently normalized:
$$\psi_\ell(k,r) = \frac{k^{\alpha+\frac{1}{2}}}{F_\ell(k)} \phi_\ell(k,r) . \tag{2.8}$$
The reason for distinguishing two regular solutions is that ϕ_ℓ has a simple boundary condition at $r = 0$, while ψ_ℓ has a *physical* boundary condition at $r \to \infty$: For $k > 0$, the representation

[2] The symmetric channel in one spatial dimension is different and must be discussed separately.

$$\psi_\ell(k,r) = \frac{i}{2}\left[f_\ell(-k,r) + e^{-(\alpha+\frac{1}{2})\pi}\frac{F_\ell(-k)}{F_\ell(k)} f_\ell(k,r)\right] \tag{2.9}$$

combined with Eq. (2.4) implies that ψ_ℓ has an asymptotic description in terms of incoming and outgoing spherical waves. The prefactor of the outgoing wave is the *scattering matrix*

$$S_\ell(k) \equiv \frac{F_\ell(-k)}{F_\ell(k)}\,. \tag{2.10}$$

From $F_\ell(-k^*) = F_\ell^*(k)$, we conclude that $S_\ell(k)$ must be a pure phase when k becomes real, and the *phase shift* $\delta_\ell(k) = \frac{1}{2i}\ln S_\ell(k)$ is thus identified with the (negative) phase of the Jost function

$$F_\ell(k) = |F_\ell(k)|\exp\left[-i\delta_\ell(k)\right] \qquad \text{for} \qquad k \in \mathbb{R}\,. \tag{2.11}$$

We list the most important analytic properties of the scattering solutions without proof. For more details the interested reader is referred to the literature [1, 2].

The regular and Jost solutions are bound by

$$\begin{aligned} |\phi_\ell(k,r)| &< C\left(\frac{r}{1+|k|r}\right)^{\alpha+\frac{1}{2}} \mathrm{e}^{r\,|\mathsf{Im}\,k|}\,, \\ |f_\ell(k,r)| &< K\left(\frac{r}{1+|k|r}\right)^{-\alpha+\frac{1}{2}} \mathrm{e}^{-r\mathsf{Im}k}\,. \end{aligned} \tag{2.12}$$

The positive constants C and K are independent of k and r. In particular, the regular solution is an *entire* function of k for all r, and the Jost solution is *holomorphic* in the upper complex k-plane, where $\mathsf{Im}\,k > 0$. For our approach, the most important quantity is the Jost function $F_\ell(k)$, which has the following properties [1, 2]:

1. the Jost function is holomorphic in the upper complex k-plane, where $\mathsf{Im}\,k > 0$;
2. the Jost function is symmetric under complex conjugation, $F_\ell(-k^*) = F_\ell^*(k)\,$;
3. the Jost function approaches unity as $|k| \to \infty$ everywhere in the upper complex k-plane. In particular, this implies $\lim\limits_{k\to\infty}\delta_\ell(k) = 0$ when $\mathsf{Im}\,k \searrow 0$;
4. the roots of the Jost function in the upper complex k-plane are simple and located on the imaginary axis, $k_j = i\kappa_i$ with $\kappa_j \in \mathbb{R}$. They correspond to the bound state energies $\omega_j = \sqrt{m^2 - \kappa_j^2}$ in the Schrödinger Eq. (2.1).

2.2 Green's Functions from Scattering Data

We now apply the technical machinery sketched in the last section to find efficient computation methods for the scattering data that enter the phase shift approach to quantum field theory. We begin with the *Green's function*, which is most commonly written in terms of the physical solution as

$$G_\ell(r,r';k) = -\frac{2}{\pi}\int_0^\infty dq\, \frac{\psi_\ell^*(q,r)\psi_\ell(q,r')}{(k+i\epsilon)^2-q^2} - \sum_j \frac{\psi_{\ell,j}(r)\psi_{\ell,j}(r')}{k^2+\kappa_j^2}\,. \tag{2.13}$$

The $i\epsilon$ prescription has been chosen such that the Green's function is meromorphic in the upper complex k-plane with simple poles at the bound state momenta $k = i\kappa_j$. However, the Green's function can also be rewritten as

$$G_\ell(r,r',k) = \frac{\phi_\ell(k,r_<)f_\ell(k,r_>)}{F_\ell(k)}(-k)^{\alpha-\frac{1}{2}}\,, \tag{2.14}$$

where $r_<$ ($r_>$) is the smaller (larger) of the arguments r and r', respectively. This expression has its (simple) poles precisely at the zeros of the Jost function, which are the imaginary bound state momenta. Thus both representations, Eqs. (2.13) and (2.14), have the same analytic structure in the upper complex k-plane, the same asymptotics as $|k| \to \infty$, and they both solve the same inhomogeneous differential equation, so they must be identical.

The form (2.14) is not yet suited for an efficient numerical evaluation. Although G_ℓ is analytic in the upper half-plane, f_ℓ and ϕ_ℓ contain pieces that oscillate for real k and exponentially decrease and increase, respectively, in the upper complex k-plane. We will eventually be interested in the case $r = r'$, whence the exponential factors in the product $f_\ell \cdot \phi_\ell$ cancel. Numerically, however, such a cancellation of large numbers is unstable and involves a substantial loss of precision. A better strategy is to factor out the dangerous exponential components with the following *ansatz*,[3]

$$\begin{aligned} f_\ell(k,r) &\equiv w_\ell(kr)g_\ell(k,r) \\ \phi_\ell(k,r) &\equiv \frac{(-k)^{-\alpha+\frac{1}{2}}}{2\alpha}\,\frac{h_\ell(k,r)}{w_\ell(kr)}\,, \end{aligned} \tag{2.15}$$

where $w_\ell(kr)$ is the free Jost solution introduced above. Notice that $g_\ell(k,r)$ is the ratio of the interacting and free Jost solution. In view of (2.7), we have the smooth limit

$$\lim_{r\to 0} g_\ell(k,r) = F_\ell(k)\,. \tag{2.16}$$

[3] For $n = 1$ and $n = 2$, the s-wave channel $\ell = 0$ is somewhat different and requires special treatment.

With these definitions,

$$G_\ell(r,r,k) = \frac{h_\ell(k,r)\, g_\ell(k,r)}{2\alpha\, g_\ell(k,0)}\,. \tag{2.17}$$

The two functions g_ℓ and h_ℓ are holomorphic in the upper complex k-plane and, most importantly, they are bounded according to

$$\begin{aligned} |g_\ell(k,r)| &\le \text{const.}\,, \\ |h_\ell(k,r)| &\le \text{const.}\, \frac{2\alpha r}{1+|k|r}\,, \end{aligned} \tag{2.18}$$

so that neither g_ℓ nor h_ℓ grow exponentially during the numerical integration. Thus the representation of the partial wave Green's function in terms of g_ℓ and h_ℓ is numerically tractable on the positive imaginary axis. After analytically continuing to $k = it$, the function $g_\ell(it,r)$ obeys

$$g_\ell''(it,r) = 2t\,\xi_\ell(tr)\, g_\ell'(it,r) + \sigma(r) g_\ell(it,r)\,, \tag{2.19}$$

with the boundary conditions

$$\lim_{r\to\infty} g_\ell(it,r) = 1 \qquad \text{and} \qquad \lim_{r\to\infty} g_\ell'(it,r) = 0\,. \tag{2.20}$$

Here the prime indicates a derivative with respect to the radial coordinate r. Using these boundary conditions, the differential equation is integrated numerically for $g_\ell(it,r)$, starting at $r=\infty$ and proceeding to $r=0$. For real τ, the function

$$\xi_\ell(\tau) \equiv -\frac{d}{d\tau} \ln\left[w_\ell(i\tau)\right] \tag{2.21}$$

entering the differential equation is real with $\lim_{\tau\to\infty} \xi_\ell(\tau) = 1$, so that $g_\ell(it,r)$ (and also $h_\ell(it,r)$ that will appear below) are manifestly real. The key ingredient for the computation of quantum corrections is the function

$$\nu_\ell(t) \equiv \lim_{r\to 0} g_\ell(it,r)\,. \tag{2.22}$$

The second function $h_\ell(it,r)$ obeys a similar equation

$$h_\ell''(it,r) = -2t\,\xi_\ell(tr)\, h_\ell'(it,r) + \left[\sigma(r) - 2t^2 \left.\frac{d\xi_\ell(\tau)}{d\tau}\right|_{\tau=tr}\right] h_\ell(it,r)\,, \tag{2.23}$$

with the boundary conditions

$$h_\ell(it,0) = 0 \qquad \text{and} \qquad h_\ell'(it,0) = 1\,. \tag{2.24}$$

This system of equations for $h_\ell(it,r)$ has to be integrated numerically from $r=0$ to $r=\infty$.

Our field theory applications will require us to compute these quantities both exactly and approximately as a Born expansion in powers of the potential. Fortunately, the computation of the Born approximations is also straightforward in this formalism. We expand the solutions to the differential Eqs.(2.19) and (2.23) about the free solutions,

$$g_\ell(it,r) = 1 + g_\ell^{(1)}(it,r) + g_\ell^{(2)}(it,r) + \cdots , \tag{2.25}$$

$$h_\ell(it,r) = 2\alpha r I_\alpha(tr) K_\alpha(tr) + h_\ell^{(1)}(it,r) + h_\ell^{(2)}(it,r) + \cdots , \tag{2.26}$$

where the superscript labels the order of the background potential $\sigma(r)$ and $I_\alpha(z)$ and $K_\alpha(z)$ are modified Bessel functions. Higher order approximations obey inhomogeneous linear differential equations with the boundary conditions

$$\lim_{r\to\infty} g_\ell^{(j)}(it,r) = 0 \quad \text{and} \quad \lim_{r\to\infty} g_\ell^{(j)\prime}(it,r) = 0, \tag{2.27}$$

$$h_\ell^{(j)}(it,0) = 0 \quad \text{and} \quad h_\ell^{(j)\prime}(it,0) = 0\,. \tag{2.28}$$

In these equations σ is the source term for $g^{(1)}$, $\sigma g^{(1)}$ is the source term for $g^{(2)}$, and so on. We thus obtain a coupled system of linear differential equations, which can be solved in a single numerical integration pass.

The differential equation system (2.19), (2.23), and its Born iterations are the central calculations needed to obtain the Green's function Eq. (2.13), which enters the energy density, and the Jost function Eq. (2.22), which enters the total energy. For computations on the real k-axis, these formulae can be rotated back to yield the variable phase approach discussed in the introduction.

2.3 Phase Shifts and Density of States

A central quantity that we will use in our investigations is the *density of states*. For a system with a discrete spectrum, the density of states in partial wave ℓ would be

$$\rho_\ell(k) = \sum_n \delta(k - k_{\ell,n})\,, \tag{2.29}$$

where $k_{\ell,n}$ are the wave numbers of the discrete solutions and the right-hand side is a sum of Dirac delta functions. To convert this result to an expression suitable for analysis in the continuum, we rewrite it as

$$\rho_\ell(k) = \lim_{\epsilon\to 0} \sum_n \frac{1}{\pi} \mathsf{Im} \frac{1}{k - k_n - i\epsilon}\,. \tag{2.30}$$

Using Eq. (2.13), we have the density of scattering states

$$\rho_\ell(k) = \frac{2k}{\pi} \mathsf{Im} \int_0^\infty dr\, G_\ell(r,r,k)\,, \tag{2.31}$$

which is valid only as a formal expression, since it contains singularities as the arguments of the Green's function coincide. As expected from Eq. (1.9), ρ_ℓ is proportional to the volume, which is infinite in the continuum limit. However, the difference between the density of states in the interacting and the free theories,

$$\rho_\ell(k) - \rho_\ell^{(0)}(k) = \frac{2k}{\pi} \operatorname{Im} \int_0^\infty dr \left(G_\ell(r,r,k) - G_\ell^{(0)}(r,r,k) \right), \tag{2.32}$$

remains finite in the continuum limit. Here $G^{(0)}$ represents the free Green's function. To make the integral on the right-hand side well defined, we require a particular prescription, which we will now explain. In doing so, we moreover relate the density of states to scattering results we have derived above. In particular, we demonstrate a key relation between the integral over space of the Green's function and the Jost function,

$$\frac{2k}{i} \int_0^\infty dr \left[G_\ell(r,r,k) - G_\ell^{(0)}(r,r,k) \right] = i \frac{d}{dk} \ln F_\ell(k) , \tag{2.33}$$

which is valid everywhere in the upper half-plane $\operatorname{Im} k > 0$, where the spatial integral is indeed well defined.

We start by differentiating the Wronskian of the Jost solution, $f_\ell(k,r)$, and the regular solution, $\phi_\ell(k', r)$ [4],

$$\frac{d}{dr} W\left[f_\ell(k,r), \phi_\ell(k',r) \right] = \left(k^2 - k'^2 \right) f_\ell(k,r) \phi_\ell(k',r), \tag{2.34}$$

where all quantities in this relation are analytic for $\operatorname{Im} k > 0$. We integrate both sides from $r = 0$ to $r = R$. Since the regular solution $\phi_\ell(k,r)$ becomes k-independent at small r, we can compute the boundary term at $r = 0$ by replacing k' with k and using the standard Wronskian,

$$W[f_\ell(k,r), \phi_\ell(k,r)] = (-k)^{\frac{1}{2}-\alpha} F_\ell(k) , \tag{2.35}$$

giving

$$W\left[f_\ell(k,R), \phi_\ell(k',R) \right] = (-k)^{\frac{1}{2}-\alpha} F_\ell(k) + \left(k^2 - k'^2 \right) \int_0^R dr\, f_\ell(k,r) \phi_\ell(k',r) . \tag{2.36}$$

Next we differentiate with respect to k, set $k' = k$, and use the representation (2.14) for the Green's function to obtain

$$\frac{(-k)^{\alpha-\frac{1}{2}}}{F_\ell(k)} W\left[\dot{f}_\ell(k,R), \phi_\ell(k,R) \right] = \frac{\alpha - \frac{1}{2}}{k} + \frac{\dot{F}_\ell(k)}{F_\ell(k)} + 2k \int_0^R dr\, G_\ell(r,r,k) , \tag{2.37}$$

where $\dot{f}_\ell(k,R) \equiv \frac{d}{dk} f_\ell(k,R)$ and $\dot{F}_\ell(k) \equiv \frac{d}{dk} F_\ell(k)$. To eliminate the first term on the right-hand side, we subtract the same equation for the non-interacting case, giving

$$\frac{(-k)^{\alpha-\frac{1}{2}}}{F_\ell(k)} W\left[\dot{f}_\ell(k,R),\phi_\ell(k,R)\right] - (-k)^{\alpha-\frac{1}{2}}\, W\left[\dot{f}_\ell^{(0)}(k,R),\phi_\ell^{(0)}(k,R)\right]$$
$$= \frac{\dot{F}_\ell(k)}{F_\ell(k)} + 2k\int_0^R dr\, \left[G_\ell(r,r,k) - G_\ell^{(0)}(r,r,k)\right]. \qquad (2.38)$$

To complete the proof of Eq. (2.33), we have to show that the left-hand side of Eq. (2.38) vanishes as $R \to \infty$. To see this, we write the boundary condition (2.4) for the Jost solution in the form

$$f_\ell(k,R) = w_\ell(kR)\,\left[1 + \mathscr{O}(R^{-1})\right], \qquad R \to \infty, \qquad (2.39)$$

which can also be inferred from the integral equation obeyed by $f_\ell(k,r)$. Differentiating with respect to k and using the asymptotics of the free Jost solution $w_\ell(kR)$,

$$\dot{w}_\ell(kR) = \frac{d}{dk}\, w_\ell(kR) = iR\; w_\ell(kR)\,\left[1 + \mathscr{O}(R^{-2})\right],$$

it is easy to show the asymptotic behavior

$$\dot{f}_\ell(k,R) = iR\, f_\ell(k,R)\,\left[1 + \mathscr{O}(R^{-2})\right]. \qquad (2.40)$$

The first term on the left-hand side of Eq. (2.38) can thus be estimated by

$$\frac{(-k)^{\alpha-\frac{1}{2}}}{F_\ell(k)}\, W[\dot{f}_\ell(k,R),\phi_\ell(k,R)] =$$
$$i\frac{(-k)^{\alpha-\frac{1}{2}}}{F_\ell(k)}\,\{R\, W[f_\ell(k,R),\phi_\ell(k,R)] -\, f_\ell(k,R)\phi_\ell(k,R)\}\,\left[1 + \mathscr{O}(R^{-2})\right]$$
$$= -i\,[R + G_\ell(R,R,k)]\,\left[1 + \mathscr{O}(R^{-2})\right], \qquad (2.41)$$

where we have used the Wronskian of f_ℓ and ϕ_ℓ and the definition of the Green's function, Eq. (2.14). Subtracting the analogous equation in the free case, the term proportional to R drops out and we are left with

$$\frac{(-k)^{\alpha-\frac{1}{2}}}{F_\ell(k)} W\left[\dot{f}_\ell(k,R),\phi_\ell(k,R)\right] - (-k)^{\alpha-\frac{1}{2}}\, W\left[\dot{f}_\ell^{(0)}(k,R),\phi_\ell^{(0)}(k,R)\right]$$
$$= -i\left[G_\ell(R,R,k) - G_\ell^{(0)}(R,R,k)\right]\,\left[1 + \mathscr{O}(R^{-1})\right]. \qquad (2.42)$$

We estimate the large-R behavior of the difference $\Delta_\ell(k,R) \equiv G_\ell(R,R,k) - G_\ell^{(0)}(R,R,k)$ from Eqs. (2.42) and (2.38),

$$-i\,\Delta_\ell(k,R)\,[1 + \mathscr{O}(R^{-1})] = \frac{\dot{F}_\ell(k)}{F_\ell(k)} + 2k\int_0^R dr\,\Delta_\ell(k,r)\,. \qquad (2.43)$$

From the bounds Eq. (2.12) we infer that the left-hand side of Eq. (2.43) is finite for any R. Thus the integral on the right-hand side must be finite, which in particular enforces $\Delta_\ell(k, R) \to 0$ in the limit $R \to \infty$ with $\mathrm{Im}k > 0$. This completes the proof of Eq. (2.33).

We can extract further information from the above integral equation. At large R, the leading order solution is $\Delta_\ell(k, R) \propto \exp(2ikR)$. This suggests the product *ansatz* $\Delta_\ell(k, R) = \widetilde{\Delta}_\ell(k, R) \exp(2ikR)$. The integral equation and the bounds, Eq. (2.12), enforce $\widetilde{\Delta}_\ell(k, R)$ to be a rational function; it cannot be an exponential. In particular on the real axis $\widetilde{\Delta}_\ell(k, R)$ must be bounded, so that $\lim_{R\to\infty} \widetilde{\Delta}_\ell(k, R) = C_\ell(k)$, where $C_\ell(k)$ is an R-independent integration constant. Therefore, we find for $k \in \mathbb{R}$,

$$\frac{\dot{F}_\ell(k)}{F_\ell(k)} + 2k \int_0^R dr \left[G_\ell(r, r, k) - G_\ell^{(0)}(r, r, k)\right] = C_\ell(k) \exp(2ikR) \left[1 + \mathscr{O}(R^{-1})\right], \tag{2.44}$$

which oscillates as $R \to \infty$. As is typical for continuum problems, we must specify that the limit where k becomes real is taken *after* computing the spatial integral to eliminate the contribution from these oscillations at the upper limit of integration. Finally we relate the Jost function to the phase shift by Eq. (2.11). Taking the imaginary part of Eq. (2.33) and using Eq. (2.30) yields the relationship between the density of states and the phase shift,

$$\frac{1}{\pi}\frac{d\delta_\ell}{dk} = \frac{2k}{\pi}\mathsf{Im} \int_0^\infty \left(G_\ell(r, r, k + i\epsilon) - G_\ell^{(0)}(r, r, k + i\epsilon)\right) dr = \rho_\ell(k) - \rho_\ell^{(0)}(k)\,. \tag{2.45}$$

We can also rewrite Eq. (2.45) as

$$\frac{2}{\pi}\int_0^\infty dr \left(\psi_\ell^*(k, r)\psi_\ell(k, r) - \psi_\ell^{(0)*}(k, r)\psi_\ell^{(0)}(k, r)\right) = \frac{1}{\pi}\frac{d\delta_\ell}{dk}\,. \tag{2.46}$$

As argued above, the momentum on the left-hand side is understood to be defined with the $i\epsilon$ prescription necessary to keep the spatial integral well defined.

2.4 Levinson's Theorem and Finite Energy Sum Rules

The renormalization program we will carry out in the next chapter will require a set of *sum rules* relating bound state and scattering data, which include and generalize Levinson's theorem, Eq. (1.11). In their basic form, they were first derived by Puff [5] and they were later re-analyzed and extended in Ref. [6]. Here, we present a derivation of these formulae, including the special case of the symmetric channel in $n = 1$ space dimensions.

The sum rules are statements about the spectrum of the Schrödinger operator in potential scattering theory. They relate information from the continuous part of the spectrum—the phase shifts—to the bound state energies:

$$\int_0^\infty \frac{dk}{\pi} k^{2p} \frac{d}{dk} \left[\delta_\ell(k)\right]_q + \sum_j (-\kappa_{\ell,j}^2)^p = 0\,. \tag{2.47}$$

Here, ℓ is the angular momentum channel and $p, q \in \mathbb{N}$ are non-negative integers with $q \geq p$. The brackets denote the q-times Born subtracted phase shift,

$$[\delta_\ell(k)]_q = \delta_\ell(k) - \sum_{i=1}^{q} \delta_\ell^{(i)}(k) \,. \tag{2.48}$$

The roots of the Jost function $F_\ell(k)$ are located on the imaginary axis at $k = i\kappa_{\ell,j}$ $(j = 1, 2, \ldots)$; they correspond to *bound states* with energies $\omega_{\ell,j} = (m^2 - \kappa_{\ell,j}^2)^{\frac{1}{2}}$.

The sum rules in Eq. (2.47) hold in *any* number of space dimensions n, as long as the scattering wavefunction vanishes at $r = 0$. The only exception is the symmetric channel in $n = 1$, where instead the *derivative* of the wavefunction vanishes at the origin. This change has a profound impact on the analytic structure of scattering data, which underlies the sum rules. We will discuss the subtleties of the symmetric channel in Sect. 2.4.3 below.

2.4.1 Overview and Simplified Derivation

To understand the origin of the sum rules, consider first the case $p = q = 0$, which is Levinson's theorem. Our starting point is the integral

$$I_\ell = \int_{-\infty}^{\infty} dk \, \frac{\dot{F}_\ell(k)}{F_\ell(k)} \,, \tag{2.49}$$

where $F_\ell(k)$ is the Jost function introduced in Eq. (2.7) via the Jost solution $f_\ell(k, r)$. From the Schrödinger equation obeyed by $f_\ell(k, r)$ and its complex conjugate, it is easily seen that $F_\ell(-k) = F_\ell^*(k)$ for real k. If we write

$$F_\ell(k) = |F_\ell(k)| \, e^{-i\delta_\ell(k)} \,,$$

it immediately follows that the modulus $|F_\ell|$ is an even function of real k, while the phase shift $\delta_\ell(k)$ is odd. The integral in Eq. (2.49) thus becomes

$$I_\ell = (-2i) \int_0^{\infty} dk \, \frac{d\delta_\ell(k)}{dk} \,.$$

On the other hand, we can also evaluate I_ℓ by contour integration in the upper complex k-plane. The integration range on the real axis is closed by a large circle in the upper complex k-plane, as shown in Fig. 2.1. Since F_ℓ has simple roots at the bound state momenta $k = i\kappa_{\ell,j}$ on the imaginary axis, the function $\dot{F}_\ell(k)/F_\ell(k)$ has simple poles with unit residue at the bound states, with no other singularities in the upper complex k-plane. In addition, $F_\ell(k)$ goes to unity at large $|k|$, so $\dot{F}_\ell(k)/F_\ell(k)$ falls off as $|k|^{-2}$ in the upper complex plane, and the semi-circle at infinity in Fig. 2.1 does not contribute. By Cauchy's theorem,

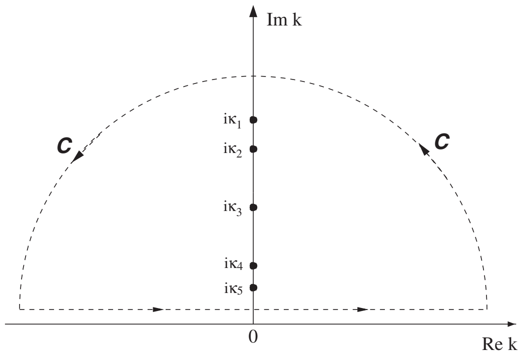

Fig. 2.1 The integration contour for Levinson's theorem and its generalizations

$$I_\ell = 2\pi i \ \mathrm{Res}\left\{\dot{F}_\ell(k)/F_\ell(k)\,;\ \mathsf{Im}\, k > 0\right\} = 2\pi i \sum_{j(\ell)} 1\,,$$

where $j(\ell)$ runs over the bound states in the ℓth partial wave. Combining the two expressions for I_ℓ gives Levinson's theorem

$$\int_0^\infty \frac{dk}{\pi}\,\frac{d\delta_\ell(k)}{dk} + \sum_{j(\ell)} 1 = 0\,, \tag{2.50}$$

or equivalently, $\delta(\infty) - \delta(0) = \pi n_\ell$, where n_ℓ is the number of bound states in channel ℓ.

It is clear that this derivation can be generalized: We could consider a starting integral with the function $\dot{F}_\ell/F_\ell$ replaced by $u(k)\,\dot{F}_\ell(k)/F_\ell(k)$, where $u(k)$ is *any* even function of k that is holomorphic in the upper complex plane. The only tricky point is to ensure that the semi-circle at infinity does not contribute; if this is the case, the general sum rule follows immediately,

$$\int_0^\infty \frac{dk}{\pi}\,u(k)\,\frac{d}{dk}\,[\delta_\ell(k)] + \sum_{j(\ell)} u(i\kappa_{\ell,j}) = 0\,. \tag{2.51}$$

The key point in the derivation of Eq. (2.47) is thus to compensate for the rise of $u(k) = k^{2p}$ by subtracting enough Born approximations from the Jost function or phase shifts, which improves the convergence at large $|k|$. In general, $q \geq p$ subtractions are required. The proof must also ensure that the Born subtractions do not interfere with the analytic structure of $\dot{F}_\ell(k)/F_\ell(k)$.

2.4.2 Proof of the Regular Sum Rules

To simplify the notation, we shall present the complete proof of the sum rules Eq. (2.47) for the *antisymmetric* channel in $n = 1$ and drop the channel index ℓ. In higher space dimensions n, the method of proof is unchanged;

some of the exponentials in the integral equations below must be replaced by Bessel functions and the corresponding bounds on the solution are slightly more complicated. Other than that, the generalization to all regular channels is straightforward.

We begin by parameterizing the Jost solution to the Schrödinger Eq. (2.1) in $n = 1$,

$$f(k,r) = \exp\left(ikr + i\beta(k,r)\right) . \tag{2.52}$$

The free Jost solutions are just plane waves e^{ikr} and the *Jost function* is $F(k) = f(k,0)$. Up to a factor of $-i$, the complex exponent $\beta(k,r)$ thus agrees with the logarithm of the Jost function. We already argued that $F(-k) = F^*(k)$ for real k. As a consequence, the (negative) phase of the Jost function—otherwise known as the *phase shift*—can be written as

$$\delta(k) = \frac{1}{2i}\left[\ln F(-k) - \ln F(k)\right] = -\mathsf{Re}\,\beta(k,0)\,. \tag{2.53}$$

To compute $\beta(k,0)$, we insert our parameterization into the Schrödinger Eq. (2.1). The result is an ordinary nonlinear differential equation

$$-i\beta''(k,r) + 2k\beta'(k,r) + \beta'^2(k,r) + \sigma(r) = 0\,, \tag{2.54}$$

where primes denote differentiation with respect to the radial coordinate, r. The scattered particle becomes free at large distances, $f(k,r) \to 1$ at $r \to \infty$. This result implies the boundary conditions

$$\beta(k,\infty) = 0 \qquad \text{and} \qquad \beta'(k,r)|_{r=\infty} = 0\,. \tag{2.55}$$

For the following, it is convenient to recast Eqs. (2.54) and (2.55) into a nonlinear integro-differential equation,

$$\beta(k,r) = \frac{1}{2k}\int_r^\infty ds\,\left(1 - e^{2ik(s-r)}\right)\Gamma(k,s), \tag{2.56}$$

where[4]

$$\Gamma(k,r) \equiv \beta'^2(k,r) + \sigma(r). \tag{2.57}$$

By differentiation, we find a similar equation for $\beta'(k,r)$,

$$\beta'(k,r) = i\int_r^\infty ds\, e^{2ik(s-r)}\Gamma(k,s). \tag{2.58}$$

Since $\beta(k,r)$ appears on both sides of these equations, we can start with $\Gamma(k,r) = \sigma(r)$ and $\beta^{(0)}(k,r) \equiv 0$ and solve for $\beta(k,r)$ by iteration. The result is a formal expansion in powers of the scattering potential $\sigma(r)$,

[4] For $n > 1$ space dimensions we merely need to modify the kernel $\Gamma(k,s)$ by a suitable combination of Bessel functions. Though similar in notation, this kernel should not be confused with (in)complete Gamma functions.

$$\beta(k,r) = \sum_{\nu=0}^{\infty} \beta^{(\nu)}(k,r)\,.$$

In view of Eq. (2.53), this expansion coincides with the usual *Born series*. The νth order Born term $\beta^{(\nu)}(k,r)$ obeys, from the iterated Eq. (2.56),

$$\beta^{(\nu)}(k,r) = \frac{1}{2k}\int_r^\infty ds\left(1-e^{2ik(s-r)}\right)\Gamma^{(\nu)}(k,s)\,. \qquad (2.59)$$

Here, $\Gamma^{(\nu)}$ denotes the term in the expansion of Γ which is of νth order in the potential $\sigma(r)$. Notice that $\sigma(r)$ only appears explicitly at level $\nu = 1$, while higher orders $\Gamma^{(\nu)}$ involve only $\beta'^{(\mu)}$ with $\mu < \nu$.

The first few Born terms from this iteration are

$$\beta^{(1)}(k) = \frac{1}{2k}\int_0^\infty ds\,\left(1-e^{2iks}\right)\sigma(s)\,,$$

$$\beta^{(2)}(k) = \frac{1}{2k}\int_0^\infty ds\,\left(1-e^{2iks}\right)[\beta'^{(1)}(k,s)]^2\,,$$

$$\beta^{(3)}(k) = \frac{1}{2k}\int_0^\infty ds\,\left(1-e^{2iks}\right)2\beta'^{(1)}(k,s)\beta'^{(2)}(k,s)\,. \qquad (2.60)$$

Similar relations can also be found for the derivatives, which appear as sources in Eqs. (2.60),

$$\beta'^{(1)}(k,r) = i\int_r^\infty ds\, e^{2ik(s-r)}\sigma(s)\,,$$

$$\beta'^{(2)}(k,r) = i\int_r^\infty ds\, e^{2ik(s-r)}[\beta'^{(1)}(k,s)]^2\,,$$

$$\beta'^{(3)}(k,r) = i\int_r^\infty ds\, e^{2ik(s-r)}2\beta'^{(1)}(k,s)\beta'^{(2)}(k,s)\,. \qquad (2.61)$$

The exponential factors in Eq. (2.59) guarantee that $\beta^{(\nu)}(k,r)$ is analytic in the upper complex k-plane provided that $\Gamma^{(\nu)}$ is, and the same holds for $\beta'^{(\nu)}(k,r)$. Starting with $\Gamma^{(1)} = \sigma(r)$, we can now derive the analytical properties of $\beta^{(\nu)}$ and $\beta'^{(\nu)}$ by induction. For instance, the large $|k|$-behavior of $\beta^{(\nu)}$ follows from the respective integral equations by a simple integration by parts, which allows to estimate the remainder using the Riemann–Lebesgue lemma. For the value at the origin, $\beta^{(\nu)}(k) \equiv \beta^{(\nu)}(k,0)$, we find:

1. If the potential $\sigma(r)$ is regular and sufficiently short-ranged [1, 2], the function $\beta^{(\nu)}(k)$ is holomorphic in the upper half-plane including $k = 0$.
2. At large momenta $|k| \to \infty$ (again in the upper complex k-plane), $\beta^{(\nu)}(k)$ decays as $|k|^{-2\nu+1}$. Similarly $\beta'^{(\nu)}(k) = \left.\frac{d\beta^{(\nu)}(k,r)}{dr}\right|_{r=0}$ decays as $|k|^{-2\nu+2}$.

Finally, we define the approximate Jost function

$$F_q(k) \equiv \exp\left[i \sum_{\nu=1}^{q} \beta^{(\nu)}(k)\right] . \tag{2.62}$$

Notice that the Born series expands the *logarithm* of the Jost function, rather than the function itself. Thus, Eq. (2.62) gives the qth order Born approximation to $F(k)$, and its (negative) phase is consequently the phase shift in qth order Born approximation. Since $\beta^{(\nu)}(-k) = -\beta^{(\nu)*}(k)$ for real k (cf. Eq. (2.54)), we can again follow our previous steps and relate the phase shift to the exponents $\beta^{(\nu)}(k)$,

$$\delta_q(k) = -\mathsf{Re} \sum_{\nu=1}^{q} \beta^{(\nu)}(k) . \tag{2.63}$$

The analytical properties of $F_q(k)$ follow directly from those of $\beta^{(\nu)}(k)$ and the convergence of the Born series $\beta(k) = \sum_{\nu=1}^{\infty} \beta^{(\nu)}(k)$ at large $|k|$ in the upper half-plane [1, 2]:

(a) the Born approximation $F_q(k)$ is analytic and has no zeros in the upper complex k-plane including $k = 0$;

(b) the difference $|\ln F(k) - \ln F_q(k)|$ falls like $|k|^{-2q-1}$ as $|k| \to \infty$ in the upper complex k-plane.

With these analytic properties of scattering data at hand, it is now easy to prove the basic sum rule Eq. (2.47) as outlined in the last section. We start with the integral

$$\begin{aligned} I_{p,q} &\equiv \int_{-\infty}^{\infty} dk\, k^{2p} \frac{d}{dk} \left[\ln F(k) - \ln F_q(k)\right] \qquad (2.64) \\ &= \int_{0}^{\infty} dk\, k^{2p} \frac{d}{dk} \left[\ln F(k) - \ln F(-k) - \ln F_q(k) + \ln F_q(-k)\right] \\ &= -2i \int_{0}^{\infty} dk\, k^{2p} \frac{d}{dk} \left[\delta(k) - \delta_q(k)\right] = -2i \int_{0}^{\infty} dk\, k^{2p} \frac{d[\delta(k)]_q}{dk} . \end{aligned}$$

This integral can also be computed by contour integration as indicated in Fig. 2.1. The analytic property (b) above ensures that the integral along the semi-circle at $|k| \to \infty$ vanishes for $q \geq p$. Moreover, $d \ln F/dk$ has simple poles of unit residue at each bound state, and $d \ln F_q/dk$ is holomorphic in the upper k-plane (property (a) above). Therefore, Cauchy's theorem gives

$$I_{p,q} = 2\pi i \ \mathrm{Res}\left\{k^{2p}\, \dot{F}(k)/F(k)\,;\, \mathsf{Im}\, k > 0\right\} = 2\pi i \sum_j (i\kappa_j)^{2p} ,$$

as long as $q \geq p$. Together with Eq. (2.64), this result proves the basic sum rules Eq. (2.47).

2.4.3 The Symmetric Channel in One Dimension

The symmetric channel in one space dimension is special since the *derivative* of the scattering wavefunction vanishes at the origin rather than the wavefunction itself. As we will see, this change leads to subtleties that can introduce anomalous contributions to the sum rules when too many subtractions are attempted:

$$\int_0^\infty \frac{dk}{\pi}\, k^{2p} \frac{d}{dk} \left[\delta(k)\right]_q = -\sum_j (-\kappa_j^2)^p + I^{\rm anom}_{p,q} \,. \tag{2.65}$$

As before, we need $q \geq p$ subtractions for the integral to converge. The anomalous term only arises when $q \geq 2p$. As a result, the "minimally subtracted" sum rules are non-anomalous, *except* for the case $p = q = 0$, which is Levinson's theorem. For that special case we will compute $I^{\rm anom}_{0,0} = \frac{1}{2}$ and recover the modified theorem in the symmetric channel [7],

$$\int_0^\infty \frac{dk}{\pi} \frac{d}{dk} \delta(k) = \frac{1}{\pi}(\delta(\infty) - \delta(0)) = \frac{1}{2} - \sum_j 1 = \frac{1}{2} - n \,. \tag{2.66}$$

This formula seems to be incorrect for the trivial case of vanishing potential. In that case, however, there exists a "half-bound" state at $k = 0$ whose wavefunction approaches a constant (rather than a generic linear function) at large distances. In the contour integration that proves the sum rules, we must then avoid the bound state pole at $k = 0$ using a small semi-circle around the origin. Thus the integral picks up *half* the usual contribution from a bound state. Such states can occur in any channel, when a state is on the threshold of binding. Since the symmetric channel in one dimension has a bound state for an arbitrarily weak attractive potential (and no bound state for an arbitrarily weak repulsive potential), the free background is an example of this otherwise exceptional situation.

Next we turn to the proof of the anomalous sum rule Eq. (2.65). The regular solution to the Schrödinger equation obeys the boundary conditions $\phi'(k, 0) = 0$ and $\phi(k, 0) = 1$. Since the scattering wavefunction $\psi(k, r)$ is proportional to it, we can represent $\psi(k, r)$ in terms of the Jost solution

$$\psi(k, r) = \frac{1}{2ki} \left[G(k) f(-k, r) - G(-k) f(k, r)\right] , \tag{2.67}$$

where $G(k) \equiv \left.\frac{df(k,r)}{dr}\right|_{r=0}$ replaces the definition in Eq. (2.7). From the defining asymptotic behavior

$$\psi(k, r) \to e^{-ikr} + e^{2i\delta(k)} e^{ikr} \quad \text{for} \quad r \to \infty, \tag{2.68}$$

we now read off the phase shift,

$$\delta(k) = \frac{1}{2i}\left[\ln(-G(-k)) - \ln G(k)\right] . \tag{2.69}$$

So far, these relations look very similar to the antisymmetric channel, with the Jost function $F(k)$ replaced by $G(k)$. Using our previous parameterization (2.52) of the Jost solution, we find

$$G(k) = i(k + \beta'(k,0))\, e^{i\beta(k,0)} . \tag{2.70}$$

We will proceed as before and compute the integral in the sum rule (2.65) by contour integration. To eliminate the large circle in the upper k-plane (cf. Fig. 2.1), the Born approximation $\ln G_q(k)$ must again be subtracted. In view of Eq. (2.70), the correct Born approximation to $G(k)$ is therefore

$$\begin{aligned} \ln G_q(k) &= \lfloor \ln(k + \beta'(k)) \rfloor_q + \ln F_q(k) + \frac{\pi}{2} \\ &= \ln(k) + \lfloor \ln(1 + \frac{\beta'(k)}{k}) \rfloor_q + \ln F_q(k) + \frac{\pi}{2} , \end{aligned} \tag{2.71}$$

where the bracket notation "$\lfloor \ldots \rfloor_q$" indicates that all terms up to order q in the background potential should be *kept*, the complement of Eq. (2.48). As we will observe, the anomaly arises because $G_q(k)$ fails to be analytic at $k = 0$; instead, the threshold pole at $k = 0$ contributes with half its residuum, which is the anomaly. This situation can arise even for $q = 0$ because of the half-bound state in the non-interacting case. Using the analytic properties of $F_q(k)$, $\beta(k,r)$, and $\beta'(k,r)$ derived in the last section, it is now easy to verify that

(a) the Born approximation $G_q(k)$ is analytic and has no zeros in the upper complex k-plane except for $k = 0$;

(b) the difference $|\ln G(k) - \ln G_q(k)|$ decays like $|k|^{-2q-1}$ at large momenta $|k|$ in the upper complex k-plane;

(c) the function $k^{2p} d \ln G_q(k)/dk$ has a simple pole with residue $2I_{p,q}^{\text{anom}}$ at $k = 0$. In the (symmetrized) contour integral this pole contributes with *half* its residue, i.e., $I_{p,q}^{\text{anom}}$;

(d) The anomaly vanishes for $2p > q$.

To complete the analysis, we compute the residue from the singularity of $G_q(k)$ at $k = 0$. Only the first term in Eq. (2.71) is potentially singular, since we already established that $\ln F_q(k)$ is analytic at $k = 0$. Thus the only part of the integrand in Eq. (2.64) (now with the replacements $F(k) \to G(k)$ and $F_q(k) \to G_q(k)$) that may be singular at $k = 0$ arises from

$$k^{2p}\frac{d}{dk}\lfloor \ln(k+\beta'(k))\rfloor_q = k^{2p}\left\lfloor \frac{1+\frac{d\beta'(k)}{dk}}{k+\beta'(k)}\right\rfloor_q$$
$$= k^{2p-1}\left\lfloor\left(1+\frac{d\beta'(k)}{dk}\right)\sum_{t=0}^{\infty}\left(\frac{-\beta'(k)}{k}\right)^t\right\rfloor_q \quad (2.72)$$

Since the functions $\beta'^{(\nu)}(k)$ are all analytic near $k=0$, an anomalous contribution to the sum rule will only result if the prefactor k^{2p-1} is overcome by the $1/k$ terms in the sum on the right-hand side of Eq. (2.72). Note that the "$\lfloor\ldots\rfloor_q$" prescription terminates the sum over t. Though the particular upper limit depends on the order at which $\beta'(k)$ is considered, we have at least $t\leq q$. The most singular term from that sum is $(-\beta'^{(1)}(k)/k)^q\sim k^{-q}$, which outweighs the prefactor k^{2p-1} if $q\geq 2p$. If $q=2p$ the singularity is a simple pole at $k=0$; for $q>2p$ there are poles of higher order as well. It is now straightforward (though increasingly tedious) to pull out the residue of the simple pole from Eq. (2.72), which is twice the anomalous contribution to the sum rule:

$$I_{p,q}^{\rm anom} = \frac{1}{2}\,{\rm Res}\left\{k^{2p-1}\left\lfloor\left(1+\frac{d\beta'(k)}{dk}\right)\sum_{t=0}^{\infty}\left(\frac{-\beta'(k)}{k}\right)^t\right\rfloor_q ; k=0\right\} . \quad (2.73)$$

Let us finally illustrate this result by looking at some important special cases:

$p=q=0$: *Levinson's Theorem*

Since the zeroth order Born approximation vanishes, $\beta^{(0)}(k,r)\equiv 0$, the residue solely arises from the prefactor, which is just $1/k$ and we have $I_{0,0}^{\rm anom}=1/2$. As mentioned above, this result is the modification of Levinson's theorem in the symmetric channel, Eq. (2.66) [7].

$p=q>0$: *Minimal Subtraction*

This is the minimal number of subtractions which will render the integral in the sum rules finite. The most singular term in the sum on the right-hand side of Eq. (2.72) (through qth order in the potential) is proportional to $(-\beta_1'(0))^q/k^{q+1}$. Combined with the prefactor the integrand in the contour integral behaves as $k^{2p-1-q}=k^{p-1}$ near $k=0$. For $p=q>0$, there is thus no threshold pole and $I_{p,p}^{\rm anom}=0$: the minimally subtracted form of the sum rules is non-anomalous.

$2p>q$: *Oversubtraction Without Anomaly*

By the same argument as above, the most singular term in the integrand now behaves as k^{2p-1-q} near $k=0$, so that no anomaly arises even for oversubtractions, as long as $q<2p$.

$q=2p$: *Computation of the Anomaly*

In this case we have $I_{p,2p}^{\rm anom}=\frac{1}{2}\left[-\beta'^{(1)}(0)\right]^{2p}$. From the integral Eqs. (2.61), we have

$$\beta'^{(1)}(0) = i\int_0^{\infty} dr\,\sigma(r),$$

so that the anomaly takes the explicit form

$$I_{p,2p}^{\text{anom}} = \frac{(-1)^p}{2} \left[\int_0^\infty dr\, \sigma(r) \right]^{2p} . \tag{2.74}$$

The first non-trivial application of this result is the $p = 1$ sum rule with two Born subtractions (i.e., one oversubtraction):

$$\int_0^\infty \frac{dk}{\pi} k^2 \frac{d}{dk} \left[\delta(k) - \delta^{(1)}(k) - \delta^{(2)}(k) \right] = \sum_j \kappa_j^2 - \frac{1}{2} \left[\int_0^\infty dr\, \sigma(r) \right]^2 . \tag{2.75}$$

This relation was first discovered in Ref. [8] by direct evaluation of the Feynman graph corresponding to the second Born approximation. Here we see that it follows from a careful analysis of the analytic properties of the Born approximation near $k = 0$.

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