A practical walk through formal scattering theory

Connecting bound states, resonances, and scattering states in exotic nuclei and beyond

Contour rotation

Sebastian König, NC State University



Virtual states

- as mentioned before, complex momenta $k=-{
 m i}\kappa$ also yield negative energies
- S-matrix poles at such positions in the complex k plane are called **virtual states** (or antibound states)



- as a function of energy, the S-matrix has multiple branches: $S_l^{\mathrm{I}}(E)$, $s_l^{\mathrm{II}}(E)$
 - \blacktriangleright bound states are poles of $S^{\mathrm{I}}_l(E)$ for negative E , $k=\mathrm{i}\kappa$
 - \blacktriangleright virtual (antibound) states are poles of $S_l^{\mathrm{II}}(E)$ for negative E, $k=-\mathrm{i}\kappa$
 - ▶ other poles of $S_l^{\mathrm{II}}(E)$ are resonances

Riemann sheets

- recall that for $E=k^2$, \sqrt{E} can equally well be defined as +k or -k
- these are the two branches of the square root function
- typically, the principal branch is taken to be the positive solution
- both branches can be combined by defining \sqrt{E} on a **Riemann surface**
 - ► in this case, it is built out of two Riemann sheets
 - ▶ these are connected at the branch cut, chosen along the negative real axis



Leonid 2, via Wikimedia commons

Analytic structure of the S-matrix

• from the square-root structure it follows that the two sheets of the S-matrix as a function *E* correspond to the upper and lower half planes as a function of *k*



Example



calculation by Nuwan Yapa

Riemann sheets of the T-matrix

 consider now the (partial-wave projected) Lippmann-Schwinger equation in momentum space:

$$T(E;p,p') = V(p,p') + \int_0^\infty rac{dq \, q^2}{2\pi^2} V(p,q) G_0(E;q) T(E;q,p')$$
 (1)

- we have written this in full off-shell form, with the energy E a free parameter not associated with either p or p'
- just like the S-matrix, the T-matrix has two Riemann sheets, which in the following we denote by T^{I} and T^{II} , and Eq. (1) is the equation for $T = T^{I}$
- that means, even if we choose E complex, we do not leave the first sheet

How then can we obtain T^{II} ?

Contour rotation

- recall that the scattering cut connects the first and second Riemann sheets
 - ▶ it runs along the positive real axis
 - ▶ this is precisely where we integrate in the Lippmann-Schwinger equation: $\int_0^\infty dq$
 - ${\scriptstyle \blacktriangleright}$ for scattering calculations, we use $i \varepsilon \rightarrow 0\,$ to approach the upper rim of the cut
- let us now deform this integration contour by rotating it into the lower half plane



• the contribution from the arc can be neglected if both V(p,q) and T(E;q,p') fall off sufficiently fast for $q \to \infty$

Analytic continuation

- to rotate the contour in the first place, we need to assume of course that the potential is actually defined for complex momenta
 - ▶ for short-range local potentials this is just fine because the integral

$$V_l(p,k) = 4\pi \int_0^\infty \mathrm{d}r\, r^2 j_l(pr) V(r) j_l(kr)$$

converges for all p and k

► so-called separable potentials, i.e., potentials that factorize as

$$V(p,k)\sim g(p)g(k)$$

are also no problem provided the "form factor" g(p) is an analytic function of p

• after rotating the contour, we can pick E with $q_0 = \sqrt{2\mu E}$ such that $-\arg q_0 < \phi$ and write down the Lippmann-Schwinger equation on the second sheet as

$$T^{\mathrm{II}}(E;p,p') = V(p,p') + \int_{\mathcal{C}_{\phi}} \frac{dq \, q^2}{2\pi^2} V(p,q) G_0(E;q) T^{\mathrm{II}}(E;q,p')$$
 (2)

Rotation reversed

- the contour-rotation method is strikingly simple, but it introduces the angle ϕ as an additional parameter in the calculation
- note now that the free Green's function for has a pole at $q=q_0=\sqrt{2\mu E}$:



- if we want to rotate the contour back to the real axis, we will sweep across this pole
- this means that we will pick up a residue contribution

for a more detailed discussion, see W. Glöckle, The Quantum Mechanical Few-Body Problem, Springer, 1983

Full circle

- let us retrace our steps so far:
- 1. without specifying the energy explicitly, we rotated the $\mathrm{d}q$ integral
- 2. we then chose the energy E in the accessible part of the second sheet
- 3. after fixing E, we rotate the integral back and pick up a residue
- this leads to the following equation:

$$egin{aligned} T^{\,\mathrm{II}}(E;p,p') &= V(p,p') + \int_0^\infty rac{dq\,q^2}{2\pi^2} V(p,q) G_0(E;q) T^{\,\mathrm{II}}(E;q,p') \ &- rac{\mathrm{i} \mu q_0}{\pi} V(p,q_0) T^{\,\mathrm{II}}(E;q_0,p') \ \end{aligned}$$

• for the new amplitude $T^{II}(E;q_0,p)$ we need a supplementary equation:

$$egin{aligned} T^{\mathrm{II}}(E;q_0,p') &= V(q_0,p') + \int_0^\infty rac{dq\,q^2}{2\pi^2} V(q_0,q) G_0(E;q) T^{\mathrm{II}}(E;q,p') \ &- rac{\mathrm{i} \mu q_0}{\pi} V(q_0,q_0) T^{\mathrm{II}}(E;q_0,p') \end{aligned}$$

Second-sheet kernel

- in numerical calculations, where we discretize the dq integral, we can combine the two equations (4) and (5) by adding q_0 as an extra mesh point
- this is similar to our numerical treatment of the principal-value integral that we encountered for scattering calculations
- a yet simpler equation can be obtained by eliminating $T^{\text{II}}(E;q_0,p')$ explicitly:

$$T^{\mathrm{II}}(E;p,p') = ilde{V}(q_0;p,p') + \int_0^\infty rac{dq \, q^2}{2\pi^2} ilde{V}(q_0;p,q) G_0(E;q) T^{\mathrm{II}}(E;q,p') \,, \quad (6)$$

with

$$ilde{V}(q_0;p,p') = V(p,p') - V(p,q_0) rac{\mathrm{i} \mu q_0 / \pi}{1 + \mathrm{i} \mu q_0 V(q_0,q_0) / \pi} V(q_0,p')$$
(7)

- this **modified kernel for the second sheet** allows us to search for virtual states and resonances
- note that in all these equations, we have $q_0=\sqrt{2\mu E}$

Second-sheet S-matrix poles

- in order to actually search for virtual states and resonances, we need to identify poles of the S-matrix on the second sheet
- as for bound states, the poles actually are poles of the T-matrix
- to find these poles, we proceed exactly as we did for bound states
- assuming the existence of simple pole at energy E^* , the second-sheet T-matrix factorizes at the pole position:

$$T^{\mathrm{II}}(E) \sim \frac{|R\rangle\langle R|}{E - E^*} \quad \text{for } E \to E^*$$
 (8)

- we use $R(p)=\langle p|R
angle$ here to denote the vertex function

1

• inserting this into the second-sheet Lippmann-Schwinger equation (6) yields the homogeneous equation

$$R(p) = \int \frac{\mathrm{d}q \, q^2}{2\pi^2} \tilde{V}(q_0; p, q) G_0(E^*; q) R(q) \,, \tag{9}$$

where now $q_0=\sqrt{2\mu E^*}$