A practical walk through formal scattering theory

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

The radial Schrödinger equation

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Configuration-space wavefunctions

- consider a scattering state with momentum k and angular quantum numbers l, m
- by spherical symmetry, its wavefunction can be composed as

$$\langle \mathbf{r} | \psi^{(+)}_{lm,p} \rangle = R_l(r) Y_{lm}(\hat{r}) = \frac{u(r)}{r} Y_{lm}(\hat{r}) \tag{1}$$

- $u(r)$ is called the reduced radial wavefunction, and it satisfies the **radial Schrödinger equation**

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{r^2} + 2\mu \left[V(r) - E_k \right] \right] u(r) = 0 \tag{2}$$

- it is customary (and convenient) to define $U(r) = 2\mu V(r)$ and rewrite Eq. (2) entirely in terms of momentum using $k^2 = 2\mu E_k$
- more generally, Eq. (2) my involce a non-local potential $V(r, r')$:

$$\rightsquigarrow \; V(r) u(r) \longrightarrow \int \mathrm{d}r' V(r, r') u(r')$$

Free radial Schrödinger equation

- in the absence of interactions, $V(r) = 0$, we are left with the **free radial Schrödinger equation**:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} + k^2\right] u(r) = 0 \tag{3}$$

  - in particular, for finite-range interactions ($V(r) = 0$ for $r > R$), this equation is exact outside the interaction range
  - for short-range interactions ($V(r) \to 0$ faster than any power law) one can still assume this free equation asymptotically
- Eq. (3) has two linearly independent solutions:
  - **Riccati-Bessel functions** $\hat{j}_l(z) = z j_l(z) \sim z^{l+1}$ for $z \to 0$ (regular)
  - **Riccati-Neumann functions** $\hat{n}_l(z) = z n_l(z) \sim z^{-l}$ for $z \to 0$ (irregular)
  - (alternative: Riccati-Bessel function of the second kind, $\hat{y}_l(z) = -\hat{n}_l(z)$)
- any solution of the full radial Schrödinger equation (2) can be written as a linear combination of $\hat{j}_l(kr)$ and $\hat{n}_l(kr)$
  - coefficients in this linear combination depend only on k

Riccati functions

- the lowest-order Riccati functions are simply $\hat{j}_0(z) = \sin(z)$ and $\hat{n}_0(z) = \cos(z)$
- for $l > 0$, both $\hat{j}_l(z)$ and $\hat{n}_l(z)$ are combinations of $\sin(z)$ and $\cos(z)$ with prefactors that are polynomials in $1/z$
- asymptotically, $\hat{j}_l(z) = \sin(z - l\pi/2)$, and similarly for $\hat{n}_l(z)$
  - note: several different phase conventions and notations in the literature
  - quoted here: Taylor, Messiah
- the Riccati-Bessel functions satisfy a simple orthogonality relation:

$$\int_0^\infty \mathrm{d}r\, \hat{j}_l(kr)\hat{j}_l(k'r) = \frac{\pi}{2}\delta(k - k') \tag{4}$$

- **Riccati-Hankel functions** are used to represent the radial parts of in- and outgoing spherical waves:

$$\hat{h}_l^{\pm}(z) = \hat{n}_l(z) \pm \mathrm{i}\hat{j}_l(z) \sim \mathrm{e}^{\mathrm{i}z} \text{ for } z \to \infty \tag{5}$$

Boundary conditions

- a boundary condition is needed to fully specify a solution of Eq. (2)
- any physical solution needs to satisfy $u(0) = 0$
  - otherwise, the full wavefunction $\langle \mathbf{r} | \psi^{(+)}_{lm,k} \rangle$ would be singular at the origin
  - this fixes $u(r)$ up to its overall normalization
  - in a numerical implementation as initial value problem, specifying the slope $u'(r)$ at $r = 0$ determines the overall amplitude
- the **normalized radial wavefunctions** $u_{l,k}(r)$ are defined as the set of solutions satisfying

$$\int_0^\infty \mathrm{d}r \, u_{l,k}(r) u_{l,k'}(r) = \frac{\pi}{2} \delta(k - k') \tag{6}$$

  - same orthogonality relation as for Riccati-Bessel functions
  - **Note:** Taylor denotes these solutions as $\psi_{l,p}(r)$ (with $p = k$)
- alternatively, one can specify the asymptotic behavior for large r
  - more relevant formally than practically
  - we'll come back to this shortly to define the so-called Jost solutions

Asymptotic behavior

- for $r \to \infty$, the normalized wavefunction can be written in the form

$$u_{l,k}(r) \sim \hat{j}_l(kr) + k f_l(k) \hat{h}_l^+(kr) \tag{7}$$

- this directly reflects the physical picture:
  - incoming plane wave component
  - scattered outgoing spherical wave
- $f_l(k)$ here is the **partial-wave scattering amplitude**, related to the **partial-wave S-matrix** $S_l(k)$ via

$$f_l(p) = \frac{S_l(k) - 1}{2\mathrm{i}k} = \frac{\mathrm{e}^{\mathrm{i}\delta_l(k)} \sin \delta_l(k)}{k} \tag{8}$$

- alternatively, using the properties of the Riccati functions, one finds that

$$u_{l,k}(r) \sim \sin\big(kr - l\pi/2 + \delta_l(k)\big) \tag{9}$$

- this explains the name of the **scattering phase shift** $\delta_l(k)$

Scattering phase shift

- assume now we have a numerical representation of $u_{l,k}(r)$ and want to extract the phase shift $\delta_l(k)$ from the asymptotic form

- in principle, we could pick a set of points r_i, each satisfying $r_i \gg R$ and fit the numerical data to $\mathcal{N} \sin\big(kr - l\pi/2 + \delta_l(k)\big)$, thus determining $\mathcal{N}$ and $\delta_l(k)$

- an easier way uses yet another way to express the asymptotic wavefunction:

$$u_{l,k}(r) \sim \hat{n}_l(kr) - \cot\delta_l(k)\hat{j}_l(kr) \tag{10}$$

- with Eq. (10) we need only find an $r_0 \gg R$ at which the wavefunction goes through zero, then

$$\cot\delta_l(k) = -\frac{\hat{n}_l(kr_0)}{\hat{j}_l(kr_0)} \tag{11}$$

- in particular, we do not actually care how our numerical solution is normalized
- r_0 is determined numerically by a **root finding algorithm**

Jupyter demo

Scattering phase shift from radial Schrödinger equation

The regular solution

- let us now consider a solution that is fully determined (including its normalization) by a boundary condition at the origin
- the so-called **regular solution** $\phi_{l,k}(r)$ of the radial Schrödinger equation satisfies

$$\phi_{l,k}(r) \sim \hat{j}_l(kr) \text{ for } r \to 0\,, \tag{12}$$

  i.e., $\lim_{r\to 0} \phi_{l,k}(r)/\hat{j}_l(kr) = 1$
- this solution is purely real because both the radial Schrödinger equation as well as the boundary condition are real

Note

- **beware of different conventions in the literature!**
- in Eq. (12) we have followed Taylor's book
  - an alternative way to write Eq. (12) is $\phi_{l,k}(0) = 0$ and $\phi'_{l,k}(0) = k$
- Newton defines a regular solution $\varphi(r)$ that satisfies $\varphi(0) = 0$ and $\varphi'(0) = 1$
  - this has the advantage of being independent of k

The Jost solutions and functions

- alternative, one can fully determine solutions by a boundary condition at infinity
- the so-called **Jost solutions** $u^{\pm}_{l,k}(r)$ are solutions of Eq. (2) that satisfy

$$\lim_{r\to\infty} \mathrm{e}^{\mp \mathrm{i}kr} u^{\pm}_{l,k}(r) = 1 \tag{13}$$

- at the origin, these are then in general not regular ($u^{\pm}_{l,k}(0) \neq 0$)
- it holds that $u^{-}_{l,k}(r) = [u^{+}_{l,k}(r)]^{*}$
- except for $p = 0$, $u^{+}_{l,k}(r)$ and $u^{-}_{l,k}(r)$ are linearly independent

  $\hookrightarrow$ regular solution can be written as linear combination of Jost solutions,

$$\phi_{l,k}(r) = a(k) u^{-}_{l,k}(r) + b(k) u^{+}_{l,k}(r) \; , \; b(k) = a(k)^{*} \tag{14}$$

- the coefficient $a(k)$ of $u^{-}_{l,k}(r)$ in Eq. (14), with a factor $\mathrm{i}/2$ taken out, is called **Jost function** and denoted by $J^{+}_{l}(k)$ in the following, and $J^{+}_{l}(k)^{*} = J^{-}_{l}(k)$
- alternatively one can introduce the Jost functions as Wronskians ($\rightarrow$ later)

S-matrix as ratio of Jost functions

- yet another way to write the normalized solution is

$$u_{l,k}(r) \underset{r\to\infty}{\sim} \frac{\mathrm{i}}{2}\left[\hat{h}_l^-(kr) + S_l(k)\hat{h}_l^+(kr)\right] \tag{15}$$

- this can now be compared to the regular solution:

$$\phi_{l,k}(r) = J_l^+(k)u_{l,k}^-(r) + J_l^-(k)^* u_{l,k}^+(r) \tag{16}$$

- it follows that

$$S_l(k) = \frac{J_l^-(k)}{J_l^+(k)} \text{ and } \phi_{l,k}(r) = J_l^+(k)u_{l,k}(r) \tag{17}$$

- for scattering calculations this is not particularly relevant, but it allows us to study the analytic continuation of the S-matrix

Analytic properties of the Jost function

- we now consider the radial Schrödinger equation for complex momenta:

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)}{r^2} - U(r) + k^2\right] u(r) = 0\ ,\ k \in \mathbb{C} \tag{18}$$

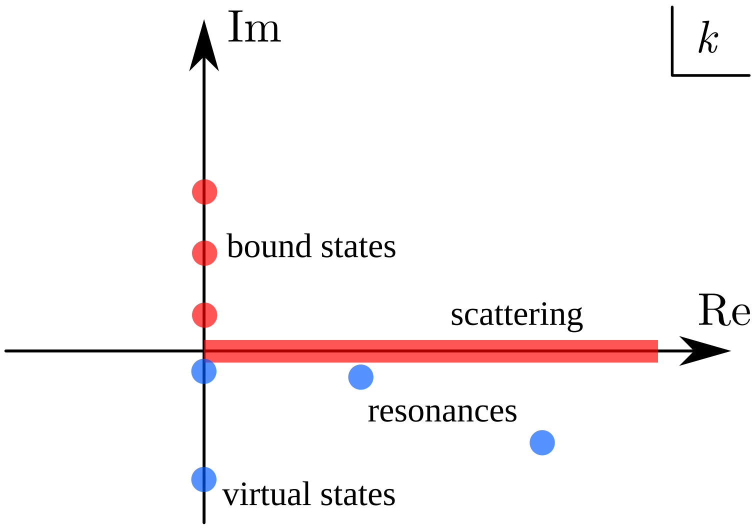
- the free solutions $\hat{j}_l(kr)$ and $\hat{n}_l(kr)$ exist for all $k \in \mathbb{C}$
  - because they are defined as power series that converge everywhere
  - in fact, they are analytic functions in k for fixed r
- based on this, it can be shown the regular solution $\phi_{l,k}(r)$ is an entire analytic function of k
- thas is, the physically relevant solutions have a **unique analytic continuation** into the complex k plane
- for the Jost functions, one finds that
  - $J_l^+(k)$ is analytic in $\mathrm{Im}\, k > 0$ and continuous in $\mathrm{Im}\, k \geq 0$
  - $J_l^+(k)^* = J_l^-(k) = J_l^+(-k)$
  - for sufficiently short ranged potentials (fall-off faster than an exponential), $J_l^+(k)$ is analytic in $\mathrm{Im}\, k < 0$ as well

The analytic S-matrix

- recall that the S-matrix is given by the ratio of Jost functions:

$$S_l(k) = \frac{J_l^-(k)}{J_l^+(k)} = \frac{J_l^+(-k)}{J_l^+(k)} \tag{19}$$

- numerator and denominator are analytic in k, but they may vanish at certain points
- therefore, the S-matrix is a **meromorphic function** on the complex k plane
  - it may have (simple) poles



Bound states

- bound states, if supported by a given potential V, are proper eigenstates with negative eigenvalues, $E < 0$
- in the complex momentum plane, they are represented by $k = \mathrm{i}\kappa$, where $\kappa > 0$ is called the binding momentum
- setting $k = -\mathrm{i}\kappa$ yields negative energies as well, this case will be discussed later
- bound-state wavefunctions are normalizable: $\displaystyle\int_0^\infty \mathrm{d}r\,|u(r)|^2 < \infty$
- based on the general form of the regular solution,

$$\phi_{l,k}(r) = J_l^+(k)u_{l,k}^-(r) + J_l^-(k)u_{l,k}^+(r)\,,$$

  we can infer that $\mathscr{F}_l(k)$ needs to vanish at $k = \mathrm{i}\kappa$, to eliminate an exponentially rising component
- the wavefunction is then directly proportional to the Jost solution $u_{l,k}^+(r)$, and

$$u(r) \underset{r\to\infty}{\sim} A\,\mathrm{e}^{-\kappa r} \tag{20}$$

Bound states as S-matrix poles

- we just derived that $J_l^+(k) = 0$ for a bound state at $k = \mathrm{i}\kappa$
- this implies that the S-matrix $S_l(k) = J_l^+(-k)/J_l^+(k)$ has a simple pole at this point in the complex k plane
- the normalized scattering wavefunction

$$u_{l,k}(r) \underset{r\to\infty}{\sim} \frac{\mathrm{i}}{2}\left[\hat{h}_l^-(kr) + S_l(k)\hat{h}_l^+(kr)\right]$$

is not defined at $k = \mathrm{i}\kappa$ due to this pole, but the regular solution

$$\phi_{l,k}(r) = J_l^+(k)u_{l,k}^-(r) + J_l^+(k)^* u_{l,k}^+(r)$$

can be analytically continued from $k > 0$ to $k = \mathrm{i}\kappa$ Fäldt+Wilkin, Physica Scripta **56** 566 (1997)

- the residue of the pole is proportional to the **asymptotic normalization constant** that appears in the bound-sate wavefunction:

$$\mathrm{Res}_{k=\mathrm{i}\kappa} S_l(p) \sim A^2 \tag{21}$$