2 Scattering theory primer

2.1 Preliminaries

Setup

- Quantum scattering of distinguishable particles 1, 2 (mass m_1, m_2)
- Hamiltonian $H = H_0 + V$ (H_0 : kinetic term, V : potential)
- Three spatial dimensions, nonrelativistic, $\hbar = 1$
- No internal degrees of freedom (spin, flavor, etc.)
- Elastic scattering (initial state = final state, no coupled channels)
- Rotational symmetry $\Leftrightarrow$ spherical potential $V(r) \Leftrightarrow [H, \boldsymbol{L}] = \boldsymbol{0}$
- Short range interaction (potential $V(r)$ vanishes at large distance $r \to \infty$ sufficiently rapidly)

Kinematics of the scattering

- Kinematics is specified by relative momentum (Fig. 8)
  - Initial state: $\boldsymbol{p}$ [in CM frame, particle 1 (2) has momentum $\boldsymbol{p}$ ($-\boldsymbol{p}$)]
  - Final state: $\boldsymbol{p}'$
- Elastic scattering does not change magnitude of momentum : $p \equiv |\boldsymbol{p}| = |\boldsymbol{p}'|$
- Two parameters which characterize scattering process
  - Scattering angle

    $$\cos\theta = \frac{\boldsymbol{p} \cdot \boldsymbol{p}'}{p^2}$$

  - Scattering energy (or momentum p)

    $$E = \frac{p^2}{2\mu}$$

    reduced mass $\mu = m_1 m_2/(m_1 + m_2)$
- Physical scattering occurs for $E > 0$, $p > 0$[1]
- Wave function is obtained by solving time-independent Schrödinger equation with energy E (§1)

[1] For physical scattering, we can use either E or p, but for the analytic continuation to complex plane, the S matrix and the scattering amplitude given below should be considered as meromorphic functions of p.

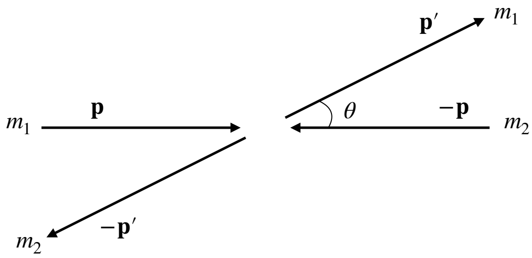

Figure 8: Schematic illustration of the kinematics of the scattering.

State vectors

- Momentum representation: initial state $|\,\boldsymbol{p}\,\rangle$, final state $\langle\,\boldsymbol{p}'\,|$, normalization is

$$\langle\,\boldsymbol{p}'\,|\,\boldsymbol{p}\,\rangle = \delta^3(\boldsymbol{p}' - \boldsymbol{p}) \tag{6}$$

  These are eigenstates of H_0 $(H_0|\,\boldsymbol{p}\,\rangle = \frac{p^2}{2\mu}|\,\boldsymbol{p}\,\rangle)$

- Angular momentum representation: initial state $|\,E,\ell,m\,\rangle$, final state $\langle\,E',\ell',m'\,|$, normalization is

$$\langle\,E',\ell',m'\,|\,E,\ell,m\,\rangle = \delta(E'-E)\delta_{\ell'\ell}\delta_{m'm} \tag{7}$$

- Relation between two:

$$\langle\,\boldsymbol{p}'\,|\,E,\ell,m\,\rangle = \frac{1}{\sqrt{\mu p}}\delta(E'-E)Y_\ell^m(\hat{\boldsymbol{p}}), \quad \hat{\boldsymbol{p}} = \frac{\boldsymbol{p}}{p} \tag{8}$$

Exercise 2

1) Using the normalization condition (6), show that the coordinate space wave function is given by $\langle\,\boldsymbol{r}\,|\,\boldsymbol{p}\,\rangle = e^{i\boldsymbol{p}\cdot\boldsymbol{r}}/(2\pi)^{3/2}$. Here the completeness relation of the coordinate basis is $1 = \int d\boldsymbol{r}|\,\boldsymbol{r}\,\rangle\langle\,\boldsymbol{r}\,|$.
2) Because $\langle\,\boldsymbol{r}\,|\,E,\ell,m\,\rangle$ is the solution without interaction, it is proportional to the spherical Bessel function and the spherical harmonics. Using the normalization condition (7), derive the expression of $\langle\,\boldsymbol{r}\,|\,E,\ell,m\,\rangle$. The spherical Bessel functions satisfy the following relation:

$$\int_0^\infty dr\ r^2 j_\ell(p'r)j_\ell(pr) = \frac{1}{2}\frac{\pi}{p^2}\delta(p'-p).$$

3) Expressing the plane wave by the spherical harmonics, show Eq. (8).

2.2 Scattering amplitude

- Scattering operator : transition from initial state to final state

$$\mathsf{S} = \Omega_-^\dagger\Omega_+ = \lim_{t\to+\infty}[e^{iH_0t}e^{-iHt}]\lim_{t\to-\infty}[e^{iHt}e^{-iH_0t}] \tag{9}$$

  $\Omega_\pm$: Møller operators

- S-matrix element (also called S matrix) : $s_\ell(E) \in \mathbb{C}$

$$\langle E', \ell', m' | \mathsf{S} | E, \ell, m \rangle = \delta(E' - E)\delta_{\ell'\ell}\delta_{m'm}s_\ell(E) \tag{10}$$

- Phase shift : $\delta_\ell(E) \in \mathbb{R}$

$$s_\ell(E) = \exp\{2i\delta_\ell(E)\} \tag{11}$$

- T matrix : $t(\boldsymbol{p}' \leftarrow \boldsymbol{p}) \in \mathbb{C}$

$$\langle \boldsymbol{p}' | (\mathsf{S} - 1) | \boldsymbol{p} \rangle = -2\pi i \delta(E' - E) t(\boldsymbol{p}' \leftarrow \boldsymbol{p})$$

- Scattering amplitude : $f(E, \theta) \in \mathbb{C}$

$$\begin{aligned} f(E,\theta) &= -(2\pi)^2 \mu \, t(\boldsymbol{p}' \leftarrow \boldsymbol{p}) \\ &= \sum_\ell (2\ell + 1) f_\ell(E) P_\ell(\cos\theta) \quad \text{(partial wave decomposition)} \end{aligned} \tag{12}$$

  Relation to S matrix

$$f_\ell(E) = \frac{s_\ell(E) - 1}{2ip} \tag{13}$$

- $s_\ell, \delta_\ell, f_\ell$ are functions of E for each ℓ

2.3 Unitarity and scattering cross section

- From definition (9), S operator is unitary (when H is hermitian)

$$\mathsf{S}^\dagger \mathsf{S} = 1$$

  Norm (probability) is conserved during time evolution

- From the completeness relation $1 = \int dE \sum_{\ell,m} | E, \ell, m \rangle \langle E, \ell, m |$ and definition (10),

$$s_\ell^*(E) s_\ell(E) = |s_\ell(E)|^2 = 1 \tag{14}$$

  This indicates that phase shift is real (when $E > 0$)

$$\exp\{2i(\delta_\ell(E) - \delta_\ell^*(E))\} = 1$$

- Scattering cross section

$$\sigma(E) = \int d\Omega |f(E,\theta)|^2 = \sum_\ell 4\pi(2\ell + 1)|f_\ell(E)|^2$$

  Substituting Eq. (13)

$$\begin{aligned} \sigma(E) &= \sum_\ell \sigma_\ell(E) \\ \sigma_\ell(E) &= \frac{2\pi(2\ell + 1)}{\mu E} \sin^2 \delta_\ell(E) \end{aligned} \tag{15}$$

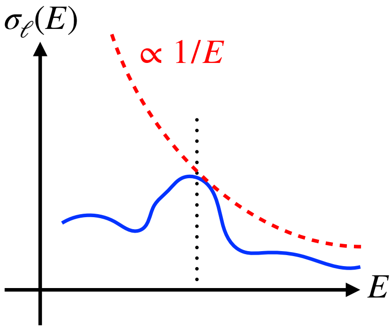

Figure 9: Schematic figure of cross section. Dashed line shows the unitarity bound $2\pi(2\ell+1)/(\mu E)$.

- Unitarity bound : because $\sin^2\delta_\ell(E) \leq 1$, cross section has upper bound (Fig. 9)

  $$\sigma_\ell(E) \leq \frac{2\pi(2\ell+1)}{\mu E}$$

  Equality holds for $\sin\delta_\ell = \pm 1$, namely, $\delta_\ell = \frac{\pi}{2}$ (modulo $\frac{\pi}{2}$)

- For $E \to 0$, upper bound of $\sigma_\ell(E)$ is ∞ (unitary limit)

2.4 Jost functions

Relation of scattering amplitude and wave function

- Riccati functions

  - 3d wave function $\psi_{\ell,m}(\boldsymbol{r})$ with $V = 0$ ($p = \sqrt{2\mu E}$) :

    $$\psi_{\ell,m}(\boldsymbol{r}) = Aj_\ell(pr) + Bn_\ell(pr) = Ch_\ell^-(pr) + Dh_\ell^+(pr)$$

    $j_\ell(z)$ $[n_\ell(z)]$: spherical Bessel (Neumann) function, $h^\pm(z)$: spherical Hankel functions

  - Radial wave function $\chi_\ell(r) \propto r\psi_{\ell,m}(\boldsymbol{r})$

  - Riccati-Bessel/Neumann function : useful to expand $\chi_\ell(r)$

    $$\hat{j}_\ell(z) = zj_\ell(z), \quad \hat{n}_\ell(z) = zn_\ell(z),$$

  - Riccati-Hankel functions

    $$\hat{h}_\ell^\pm(z) = zh_\ell^\pm(z) \to \exp\{\pm i(z - \ell\pi/2)\} \quad z \to \infty \tag{16}$$

    Namely, $\hat{h}_\ell^+(pr) \sim e^{+ipr}$ $[\hat{h}_\ell^-(pr) \sim e^{-ipr}]$ is outgoing (incoming) wave

- Regular solution $\phi_{\ell,p}(r)$: $\chi_\ell(r)$ with eigenmomentum p normalized as

  $$\frac{\phi_{\ell,p}(r)}{\hat{j}_\ell(pr)} \to 1 \quad (r \to 0) \tag{17}$$

  In addition to $\phi_{\ell,p}(r) \to 0$, its normalization is fixed

- Asymptotic form of $\phi_{\ell,p}(r)$ at $r \to \infty$: superposition of Riccati functions because of $V = 0$

$$\phi_{\ell,p}(r) \to \frac{i}{2}\left[\mathscr{f}_\ell(p)\hat{h}_\ell^-(pr) - \mathscr{f}_\ell(-p)\hat{h}_\ell^+(pr)\right] \quad (r \to \infty)$$

- Jost function $\mathscr{f}_\ell(p)$: amplitude of incoming wave ← Eq. (16)
  Amplitude of outgoing wave is given by the same function with substitution of $-p$

- **Outgoing boundary condition = zero of Jost function** $\mathscr{f}_\ell(p)$

- Jost function is an analytic function of p (∼ having no singularity)[2]

- Expansion of $\mathscr{f}_\ell(p)$ for small p : shown by integral representation

$$\mathscr{f}_\ell(p) = 1 + \underbrace{[\alpha_\ell + \beta_\ell p^2 + \mathcal{O}(p^4)]}_{\text{even powers of } p} + i\underbrace{[\gamma_\ell p^{2\ell+1} + \mathcal{O}(p^{2\ell+3})]}_{\text{odd powers of } p}, \quad \alpha_\ell, \beta_\ell, \gamma_\ell, \dots \in \mathbb{R} \tag{18}$$

- Complex conjugate of Jost function ← Eq. (18)

$$\left[\mathscr{f}_\ell(p)\right]^* = \mathscr{f}_\ell(-p^*) \tag{19}$$

Example

- s-wave case ($\ell = 0$) : $\hat{j}_0(pr) = \sin(pr)$, $\hat{h}_0^\pm(pr) = e^{\pm ipr}$

- Solution (3) of square well potential in §1.3

$$\chi(r) \to C\sin(kr) = Ckr + \mathcal{O}(r^3)$$

- Normalization of Eq. (17) : from $\hat{j}_0(pr) = pr + \mathcal{O}(r^3)$

$$\phi_{\ell,p}(r) = \chi(r)\Big|_{C=\frac{p}{k}}$$

- Jost function of square well potential

$$\frac{i}{2}\mathscr{f}_\ell(p) = A^-(p)\Big|_{C=\frac{p}{k}}$$
$$\mathscr{f}_\ell(p) = \left[\cos(kb) - i\frac{p}{k}\sin(kb)\right]e^{ipb}$$

  This follows expansion (18) for $p \to 0$, and we obtain $A^+(p) = -\frac{i}{2}\mathscr{f}_\ell(-p)$ with $C = \frac{p}{k}$

[2]Strictly speaking, region of analyticity in complex p plane is determined by the behavior of the potential.

3 Resonances in scattering theory

3.1 Resonances as poles of scattering amplitude

- §1 : resonances are discrete eigenstates of Hamiltonian (complex p) $\leftarrow$ outgoing boundary condition
- §2 : outgoing boundary condition in scattering theory is zero of Jost function $\not{f}_\ell(p) = 0$
- S matrix : amplitude of outgoing wave normalized by that of incoming wave

  $$s_\ell(p) = \frac{\text{amplitude of outgoing wave}}{\text{amplitude of incoming wave}} = \frac{\not{f}_\ell(-p)}{\not{f}_\ell(p)}$$

  $\Rightarrow$ discrete eigenstates are represented by **poles of S matrix**

- From Eq. (19), unitarity condition (14) follows

  $$s^*_\ell(p)s_\ell(p) = \frac{[\not{f}_\ell(-p)]^*}{[\not{f}_\ell(p)]^*}\frac{\not{f}_\ell(-p)}{\not{f}_\ell(p)} = \frac{\not{f}_\ell(p^*)}{\not{f}_\ell(-p^*)}\frac{\not{f}_\ell(-p)}{\not{f}_\ell(p)} = 1 \quad (p > 0)$$

  instead, $s^*_\ell(p)s_\ell(p) \neq 1$ for $p \notin \mathbb{R}$

- Scattering amplitude : from Eq. (13)

  $$f_\ell(p) = \frac{s_\ell(p) - 1}{2ip} = \frac{\not{f}_\ell(-p) - \not{f}_\ell(p)}{2ip\not{f}_\ell(p)} \tag{20}$$

  $\Rightarrow$ discrete eigenstates are represented by **poles of scattering amplitude**

- $s_\ell(p)$ and $f_\ell(p)$ are meromorphic functions of p ($\sim$ no singularity except for poles)

3.2 Eigenenergies and Riemann sheets

- Analytic continuation of $\not{f}_\ell(p)$, $s_\ell(p)$, $f_\ell(p)$ defined in physical region $p > 0$ to complex plane
- Complex momentum p, complex energy E

  $$p = |p|e^{i\theta_p}, \quad E = |E|e^{i\theta_E}$$

- Relations

  $$E = \frac{p^2}{2\mu} = \frac{|p|^2}{2\mu}e^{2i\theta_p}$$

  $$\Rightarrow \quad |E| = \frac{|p|^2}{2\mu}, \quad 2\theta_p = \theta_E$$

  - When θ_p varies $0 \to 2\pi$, θ_E moves $0 \to 4\pi$
  - p and $-p$ (θ_p and $\theta_p + \pi$) are mapped onto the same E

- Meromorphic functions of p ($s_\ell(p)$, $f_\ell(p)$) are defined on two-sheeted Riemann surface of E
  $0 \leq \theta_E < 2\pi$: 1st Riemann sheet of E (upper half plane of p, $0 \leq \theta_p < \pi$)
  $2\pi \leq \theta_E < 4\pi$: 2nd Riemann sheet of E (lower half plane of p, $\pi \leq \theta_p < 2\pi$)

- Complex p and E planes : Fig. 10
  Cut on real axis of E plane (branch point at $E = 0$)

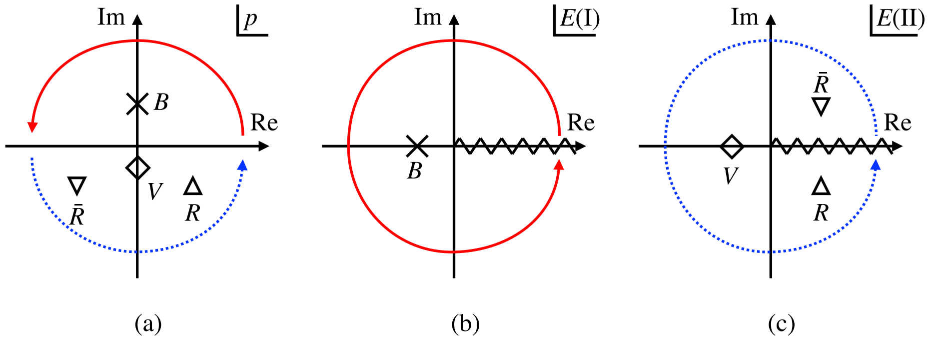

Figure 10: Poles in complex plane. (a) : p plane, (b) : E plane (1st Riemann sheet), (c) : E plane (2nd Riemann sheet). B, V, R, and $\bar{R}$ represent bound state, virtual state, resonance, and Anti-resonance.

3.3 Classification of eigenstates

- Eigenstate of Hamiltonian : zero of Jost function $\not{f}_\ell(p) = 0$
- From Eq. (19), when $\not{f}_\ell(p) = 0$,

  $$\not{f}_\ell(-p^*) = [\not{f}_\ell(p)]^* = 0$$

  $\Rightarrow$ If p is a solution, $-p^*$ (point which is symmetric about imaginary axis) is also a solution
- Solutions with $p = -p^*$ (on imaginary axis)
  - bound state (B) : $\times$ in Fig. 10

    $$\mathrm{Re}\,[p_B] = 0, \quad \mathrm{Im}\,[p_B] > 0$$

    Energy E_B is real and negative (1st Riemann sheet)
  - Virtual state (anti-bound state, V) : $\diamondsuit$

    $$\mathrm{Re}\,[p_V] = 0, \quad \mathrm{Im}\,[p_V] < 0$$

    Energy E_V is real and negative (2nd Riemann sheet)
    Residue of pole ($\sim$ norm) is negative : non-physical degree of freedom?[26]
- Solutions with $p \neq -p^*$ (always appear in pairs)
  - Solutions exist only in lower half plane of p
    $\leftarrow$ complex E is allowed only when wave function is not square integrable
  - Resonance (R) : $\triangle$

    $$\mathrm{Re}\,[p_R] > 0, \quad \mathrm{Im}\,[p_R] < 0$$

    Energy $\mathrm{Re}\,[E_R] > 0$, $\mathrm{Im}\,[E_R] < 0$ (2nd Riemann sheet)

– Anti-resonance ($\bar{R}$) : $\bigtriangledown$

$$\text{Re}\,[p_{\bar{R}}] < 0, \quad \text{Im}\,[p_{\bar{R}}] < 0$$

appears together with resonance
Growing solution with time [27] ("conjugate" of resonance)

3.4 Resonances and observables

- Only real energies are experimentally accessible
- Effect on observables by resonance pole at $E = E_R = M_R - i\Gamma_R/2$ in partial wave ℓ
- Laurent expansion of scattering amplitude around $E = E_R$

$$f_\ell(E) = f_{\ell,\text{BW}}(E) + f_{\ell,\text{BG}}(E), \tag{21}$$

Breit-Wigner term $f_{\ell,\text{BW}}(E)$: contribution from resonance pole

$$f_{\ell,\text{BW}}(E) = \frac{Z_R}{E - E_R} = \frac{Z_R(E - M_R - i\Gamma_R/2)}{(E - M_R)^2 + \Gamma_R^2/4}, \quad Z_R = -\frac{\Gamma_R}{2p_R} \tag{22}$$

Nonresonant background $f_{\ell,\text{BG}}(E)$: analytic at $E = E_R$

$$f_{\ell,\text{BG}}(E) = \sum_{n=0}^{\infty} C_n (E - E_R)^n. \tag{23}$$

- At real energy $E \sim M_R$, contribution from $f_{\ell,\text{BW}}(E)$ increases (in particular, narrow Γ_R case)
- When $f_{\ell,\text{BG}}(E)$ is **assumed** to be small and negligible

$$f_\ell(E) \approx f_{\ell,\text{BW}}(E) \quad (f_{\ell,\text{BG}}(E) \to 0). \tag{24}$$

- Resonance phenomena for real energy
(valid only when $f_{\ell,\text{BG}}(E)$ is neglected)

  (i) Re $[f_\ell(E)] = 0$ and Im $[f_\ell(E)]$ becomes maximum at $E = M_R$
  $\leftarrow Z = -\Gamma_R/(2p) < 0$ and Eq. (22) (residue Z is given on the real axis)

  (ii) cross section $\sigma(E)$ peaks at $E = M_R$
  $\leftarrow$ (i) and optical theorem (See Exercise 3)

  (iii) phase shift $\delta_\ell(E)$ increases rapidly and crosses $\frac{\pi}{2}$ at $E = M_R$
  $\leftarrow$ From Eq. (13), Im $[s_\ell(M_R)] = 0$ when Re $[f_\ell(M_R)] = 0$
  Except for the non-interacting case ($\delta_\ell = 0$), we have $\delta_\ell = \frac{\pi}{2}$ (modulo π) for Im $[s_\ell(M_R)] = 0$

- When $f_{\ell,\text{BG}}(E)$ is nonnegligible, interference term contributes

$$|f_\ell(E)|^2 = |f_{\ell,\text{BW}}(E)|^2 + |f_{\ell,\text{BG}}(E)|^2 + 2\text{Re}\,[f_{\ell,\text{BW}}(E) f^*_{\ell,\text{BG}}(E)], \tag{25}$$

- Peaks can be generated kinematically by cusps and triangle singularities [28]
- Importance of accurate analysis to determine resonance pole instead of simply fitting peak

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Exercise 3

1) Express $f_\ell(E)$ in terms of $\sin\delta_\ell(E)$ and $\cos\delta_\ell(E)$.
2) Show Eq. (15).
3) Show the following optical theorem :

$$\mathrm{Im}\ f(E,\theta=0)=\frac{p}{4\pi}\sigma(E).$$

4) Argue that the optical theorem is violated when the time evolution is not unitary.

3.5 Effective range expansion

- Low-energy (small p) behavior of scattering amplitude $f_\ell(p)$

$$\begin{aligned} f_\ell(p) &= \frac{s_\ell(p)-1}{2ip} \qquad \leftarrow (13) \\ &= \frac{p^{2\ell}}{p^{2\ell+1}\cot\delta_\ell(p)-ip^{2\ell+1}} \end{aligned} \tag{26}$$

- From Eq. (18), Jost function is written as

$$\not{f}_\ell(p)=F_\ell(p^2)+ipG_\ell(p^2)$$

F_ℓ and G_ℓ are functions of p^2 and behave at $p\to 0$ as

$$F_\ell(p^2)=\mathcal{O}(p^0),\quad G_\ell(p^2)=\mathcal{O}(p^{2\ell})$$

From this,

$$\not{f}_\ell(-p)=F_\ell(p^2)-ipG_\ell(p^2)$$

- From Eq. (20)

$$\begin{aligned} f_\ell(p) &= \frac{\not{f}_\ell(-p)-\not{f}_\ell(p)}{2ip\not{f}_\ell(p)} \\ &= \frac{p^{2\ell}}{-p^{2\ell}F_\ell(p^2)/G_\ell(p^2)-ip^{2\ell+1}} \end{aligned} \tag{27}$$

- Comparison of Eqs. (26) and (27)

$$p^{2\ell+1}\cot\delta_\ell(p)=-p^{2\ell}\frac{F_\ell(p^2)}{G_\ell(p^2)} \tag{28}$$

Right-hand-side is a function of p^2 with $\mathcal{O}(p^0)$ for $p\to 0$: Taylor expansion reads

$$\Rightarrow \quad p^{2\ell+1}\cot\delta_\ell(p)=-\frac{1}{a_\ell}+\frac{r_\ell}{2}p^2+\mathcal{O}(p^4) \tag{29}$$

which is called effective range expansion

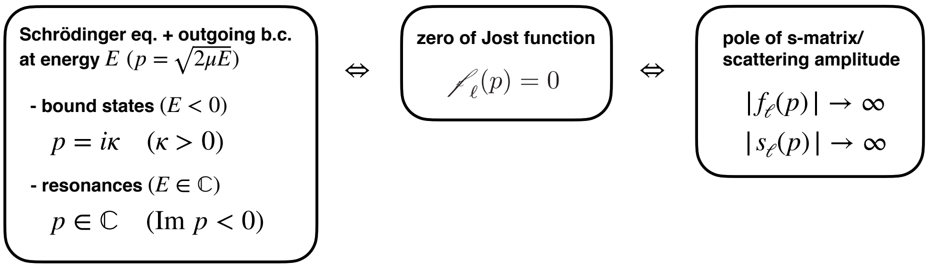

Figure 11: Various conditions for resonances. The outgoing boundary condition of the wave function is related to the pole of the scattering amplitude through the zero of the Jost function.

- s-wave case ($\ell = 0$)

$$f_0(p) = \frac{1}{-\frac{1}{a_0} + \frac{r_0}{2}p^2 + \mathcal{O}(p^4) - ip}$$

  - a_0 : scattering length, opposite sign convention is also used in hadron physics
  - r_0 : effective range, roughly corresponds to the interaction range, but can be negative
  - Eq. (28) can have a pole (CDD pole [29])
    When CDD pole exists at low energy, Padé approximant is useful [20]

- Low-energy scattering : assuming higher order terms of p is negligible

$$f_0(p) \approx \frac{1}{-\frac{1}{a_0} - ip}$$

  Pole at $p = \frac{i}{a_0}$

  - $a_0 > 0$: pole in the upper-half plane, bound state
  - $a_0 < 0$: pole in the lower-half plane, virtual state

  In both cases, energy is $E = -\frac{1}{2\mu a_0^2}$

3.6 Summary of §2 and §3

- Definition of S matrix, phase shift, scattering amplitude, etc.
- Correspondence between pole of scattering amplitude and resonance state (Fig. 11)
- Effective range expansion : description of low-energy scattering