3 Scattering theory primer

3.1 Preliminaries

- Simplest setup
  - Quantum scattering of distinguishable particles 1, 2 (mass m_1, m_2)
  - Hamiltonian $H = H_0 + V$ (H_0 : kinetic term, V : potential)
  - Nonrelativistic system in three spatial dimensions.
  - No internal degrees of freedom (spin, flavor, etc.)
  - Elastic scattering (initial state = final state, no coupled channels)
  - Rotational symmetry ⇔ spherical potential $V(r)$ ⇔ $[H, \boldsymbol{L}] = \boldsymbol{0}$
  - Short range interaction ($V(r)$ vanishes at $r \to \infty$ sufficiently rapidly)
- Kinematics ← relative momentum (Fig. 6)
  - Initial state: $\boldsymbol{p}$ [in CM frame, particle 1 (2) has momentum $\boldsymbol{p}$ ($-\boldsymbol{p}$)]
  - Final state: $\boldsymbol{p}'$

  Elastic scattering → magnitude is unchanged: $p \equiv |\boldsymbol{p}| = |\boldsymbol{p}'|$
- **Two** parameters which characterize the scattering process
  - Scattering angle θ

    $$\cos\theta = \frac{\boldsymbol{p} \cdot \boldsymbol{p}'}{p^2} \tag{19}$$
  - Scattering energy E (or momentum p)

    $$E = \frac{p^2}{2\mu} \tag{20}$$

    with the reduced mass $\mu = m_1 m_2/(m_1 + m_2)$
- Physical scattering occurs for $E > 0$, $p > 0$[2]
- Wavefunction ← time-independent Schrödinger equation for energy E (§2)

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[2] For physical scattering, either E or p can be used. However, for analytic continuation to the complex plane, the S matrix and the scattering amplitude introduced below should be regarded as meromorphic functions of p.

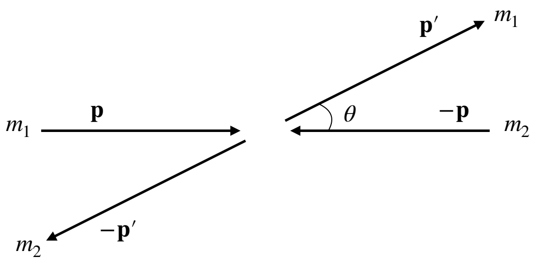

Figure 6: Schematic illustration of the kinematics of the scattering.

- Initial state $|\boldsymbol{p}\rangle$ and final state $\langle\boldsymbol{p}'|$: eigenstates of H_0 with the normalization

$$\langle\boldsymbol{p}'|\boldsymbol{p}\rangle = \delta^3(\boldsymbol{p}'-\boldsymbol{p}), \quad H_0\,|\boldsymbol{p}\rangle = \frac{p^2}{2\mu}\,|\boldsymbol{p}\rangle \tag{21}$$

  With the normalization $1 = \int d\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\langle\boldsymbol{r}|$, the wavefunction is $\langle\boldsymbol{r}|\boldsymbol{p}\rangle = e^{i\boldsymbol{p}\cdot\boldsymbol{r}}/(2\pi)^{3/2}$

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

$$\langle E',\ell',m'|E,\ell,m\rangle = \delta(E'-E)\delta_{\ell'\ell}\delta_{m'm} \tag{22}$$

- Relation between two vectors:

$$\langle\boldsymbol{p}'|E,\ell,m\rangle = \frac{1}{\sqrt{\mu p}}\delta\left(\frac{(p')^2}{2\mu}-E\right)Y_\ell^m(\hat{\boldsymbol{p}}') \tag{23}$$

3.2 Scattering amplitude

- Scattering operator: transition from initial state to final state

$$\mathsf{S} = \Omega_-^\dagger\Omega_+ = \lim_{t\to+\infty}[e^{iH_0t}e^{-iHt}]\lim_{t\to-\infty}[e^{iHt}e^{-iH_0t}] \tag{24}$$

  $\Omega_\pm$: Møller operators

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

$$\langle E',\ell',m'|\,\mathsf{S}\,|E,\ell,m\rangle = \delta(E'-E)\delta_{\ell'\ell}\delta_{m'm}s_\ell(E) \tag{25}$$

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

$$s_\ell(E) = \exp\{2i\delta_\ell(E)\} \tag{26}$$

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

$$\langle\boldsymbol{p}'|\,(\mathsf{S}-1)\,|\boldsymbol{p}\rangle = -2\pi i\delta(E'-E)t(\boldsymbol{p}'\leftarrow\boldsymbol{p}) \tag{27}$$

- **Scattering amplitude**: $f(E,\theta) \in \mathbb{C}$ (with the present convention)

$$f(E,\theta) = -(2\pi)^2\mu\, t(\boldsymbol{p}' \leftarrow \boldsymbol{p})$$
$$= \sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(E)P_\ell(\cos\theta) \quad \text{(partial wave decomposition)} \tag{28}$$

  Relation to S matrix

$$f_\ell(E) = \frac{s_\ell(E)-1}{2ip} \tag{29}$$

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

3.3 Unitarity and scattering cross section

- From definition (24), S operator is **unitary** (when H is Hermitian)

$$\mathsf{S}^\dagger\mathsf{S} = 1 \tag{30}$$

  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 (25),

$$s_\ell^*(E)s_\ell(E) = |s_\ell(E)|^2 = 1 \tag{31}$$

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

$$\exp\{2i(\delta_\ell(E) - \delta_\ell^*(E))\} = 1 \quad \Rightarrow \quad \text{Im}\ \delta_\ell(E) = 0 \tag{32}$$

- Scattering cross section

$$\sigma(E) = \int d\Omega |f(E,\theta)|^2 = \sum_\ell 4\pi(2\ell+1)|f_\ell(E)|^2 \tag{33}$$

  Substituting Eq. (29),

$$\sigma(E) = \sum_{\ell=0}^{\infty}\sigma_\ell(E) \tag{34}$$

$$\sigma_\ell(E) = \frac{2\pi(2\ell+1)}{\mu E}\sin^2\delta_\ell(E) \tag{35}$$

- **Unitarity bound**: Since $\sin^2\delta_\ell(E) \leq 1$, cross section has an upper bound (Fig. 7)

$$\sigma_\ell(E) \leq \frac{2\pi(2\ell+1)}{\mu E} \tag{36}$$

  The equality is achieved when $\sin\delta_\ell = \pm 1$, namely, $\delta_\ell = \frac{\pi}{2}$ (modulo π)

- For $E \to 0$, the upper bound of $\sigma_\ell(E)$ diverges (unitarity limit)

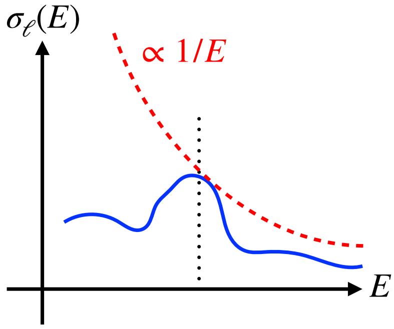

Figure 7: Schematic figure of cross section. Dashed line shows the unitarity bound $2\pi(2\ell{+}1)/(\mu E)$.

3.4 Jost functions

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

    $$\psi_{\ell,m}(\boldsymbol{r}) = [Aj_\ell(pr) + Bn_\ell(pr)]Y_\ell^m(\hat{\boldsymbol{r}}) = [Ch_\ell^-(pr) + Dh_\ell^+(pr)]Y_\ell^m(\hat{\boldsymbol{r}}) \tag{37}$$

    $j_\ell(z)$ $[n_\ell(z)]$: spherical Bessel (Neumann) function, $h_\ell^\pm(z)$: spherical Hankel functions[3]
  - Riccati-Bessel/Neumann function: useful to expand radial wave function $u_\ell(r) \propto r\psi_{\ell,m}(\boldsymbol{r})$

    $$\hat{j}_\ell(z) = zj_\ell(z), \quad \hat{n}_\ell(z) = zn_\ell(z), \tag{38}$$
  - Riccati-Hankel functions

    $$\hat{h}_\ell^\pm(z) = zh_\ell^\pm(z) \to \exp\{\pm i(z-\ell\pi/2)\} \quad z\to\infty \tag{39}$$

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

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

  $$\frac{\phi_{\ell,p}(r)}{\hat{j}_\ell(pr)} \to 1 \quad (r\to 0) \tag{40}$$

  Together with $\phi_{\ell,p}(r) \to 0$ at $r=0$, this fixes the normalization (derivative).

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

  $$\phi_{\ell,p}(r) \to \frac{i}{2}\left[\mathscr{f}_\ell(p)\hat{h}_\ell^-(pr) - [\mathscr{f}_\ell(p)]^*\hat{h}_\ell^+(pr)\right] \quad (r\to\infty) \tag{41}$$

  Since the radial Schrödinger equation does not contain i and the slope at the origin is real, $\phi_{\ell,p}(r)$ is real. $\Rightarrow D = C^*$ $([\hat{h}^\pm(z)]^* = \hat{h}^\mp(z))$ for $\phi_{\ell,p}(r) = C\hat{h}_\ell^-(pr) + D\hat{h}_\ell^+(pr)$

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[3] The definition of the Neumann function often includes a minus sign, e.g., $n_0(z) = -\cos z/z$. In scattering theory, however, the convention $n_0(z) = +\cos z/z$ is frequently used [16].

- **Jost function** $\mathscr{f}_\ell(p)$: coefficient of incoming wave ← Eq. (39)

$$\mathscr{f}_\ell(p) = 1 + \frac{2\mu}{p}\int_0^\infty dr\, \hat{h}_\ell^+(pr)V(r)\phi_{\ell,p}(r), \tag{42}$$

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

- Jost function is an analytic function of p (∼ having no singularity)[4]

- Expansion of $\mathscr{f}_\ell(p)$ for small p: shown by integral representation (42)

$$\mathscr{f}_\ell(p) = 1 + \underbrace{[\alpha_\ell + \beta_\ell p^2 + \mathcal{O}(p^4)]}_{\text{even powers of } p} + i\underbrace{[\gamma_\ell p^{2\ell+1} + \mathcal{O}(p^{2\ell+3})]}_{\text{odd powers of } p}, \quad \alpha_\ell, \beta_\ell, \gamma_\ell, \cdots \in \mathbb{R} \tag{43}$$

- Complex conjugate of Jost function ← Eq. (43)

$$[\mathscr{f}_\ell(p)]^* = \mathscr{f}_\ell(-p^*) \tag{44}$$

⇒ For physical scattering ($p > 0$),

$$\phi_{\ell,p}(r) \to \frac{i}{2}\left[\mathscr{f}_\ell(p)\hat{h}_\ell^-(pr) - \mathscr{f}_\ell(-p)\hat{h}_\ell^+(pr)\right] \quad (r \to \infty) \tag{45}$$

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

- Solution (12) of square-well potential in §2.3

$$u_0(r) \to C\sin(kr) = Ckr + \mathcal{O}(r^3) \tag{46}$$

- Normalization of Eq. (40) : from $\hat{j}_0(pr) = pr + \mathcal{O}(r^3)$

$$\phi_{\ell,p}(r) = u_0(r)\Big|_{C=\frac{p}{k}} \tag{47}$$

- Jost function of square-well potential

$$\frac{i}{2}\mathscr{f}_0^{\text{well}}(p) = A^-(p)\Big|_{C=\frac{p}{k}} \tag{48}$$

$$\mathscr{f}_0^{\text{well}}(p) = \left[\cos(kb) - i\frac{p}{k}\sin(kb)\right]e^{ipb} \tag{49}$$

This expression follows the expansion (43) for small p ⇒ $A^+(p) = -\frac{i}{2}\mathscr{f}_\ell(-p)$ with $C = \frac{p}{k}$.

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[4] Strictly speaking, region of analyticity in complex p plane is determined by the behavior of the potential with Eq. (42).