10.10.2018

Lippmann-Schwinger equation (Sakurai. P390 - P394)

Derivation:
- finite range of potential
- two wavefunctions / equations
- add together
- inverse after introducing $E \to E \pm i\varepsilon$

forwards / backwards propagating

→ LS-equation in coordinate representation:

$$\langle \vec{r} | \psi \rangle = \langle \vec{r} | \phi \rangle + \int d^3 r' \langle \vec{r} | \frac{1}{E - \hat{H}_0 + i\varepsilon} | \vec{r}' \rangle \langle \vec{r}' | \hat{V} | \psi^{\pm} \rangle$$

The kernel of the integral equation:

$$G_{\pm}(\vec{r}, \vec{r}') = \frac{\hbar^2}{2m} \langle \vec{r} | \frac{1}{E - \hat{H}_0 \pm i\varepsilon} | \vec{r}' \rangle$$

↳ represented in momentum.

$$= \frac{\hbar^2}{2m} \iint d^3p' d^3p'' \langle \vec{r} | \vec{p}' \rangle \underbrace{\langle \vec{p}' | \frac{1}{E - \hat{H}_0 \pm i\varepsilon} | \vec{p}'' \rangle}_{\frac{\delta(\vec{p}' - \vec{p}'')}{E - p^2/2m \pm i\varepsilon}} \langle \vec{p}'' | \vec{r} \rangle$$

$$\Rightarrow G_{\pm}(\vec{r}, \vec{r}') = \frac{1}{(2\pi)^3} \int d\Omega_{k'} \int_0^{\infty} dk' \frac{\exp(i|\vec{r} - \vec{r}'| k' \cos\theta)}{k^2 - k'^2 \pm i\varepsilon} k'^2$$

$$= \frac{1}{4\pi^2 i} \frac{1}{|\vec{r} - \vec{r}'|} \int_0^{\infty} dk' \frac{\exp(i|\vec{r} - \vec{r}'| k') - \exp(-i|\vec{r} - \vec{r}'| k')}{k^2 - k'^2 \pm i\varepsilon}$$

$$= -\frac{1}{4\pi} \frac{\exp(\pm ik|\vec{r} - \vec{r}'|)}{|\vec{r} - \vec{r}'|}$$

+ : outgoing

− : ingoing

$$(\vec{\nabla}^2 + k^2) G_{\pm}(\vec{r}, \vec{r}') = \delta(\vec{r} - \vec{r}')$$

15. 10. 2018

Lippmann-Schwinger-eq. (II). (Sakurai. P 394 - 397)

Solid angle: projection of one point onto sphere. We seek a physical quantity independent of distance.

$\rightarrow d\Omega = \sin\theta \, d\theta \, d\varphi$

Differential scattering cross section:

$$\left(\frac{d\sigma}{d\Omega}\right) d\Omega = \frac{r^2 |\vec{j}_{\text{scattering}}| \, d\Omega}{|\vec{j}_{in}|} = |f(\vec{k}, \vec{k}')|^2 \, d\Omega$$

$$\frac{d\sigma}{d\Omega} = |f(\vec{k}, \vec{k}')|^2 \, d\Omega$$ ← Memorise!

$$\vec{j} := \frac{\hbar}{2mi}\left(\psi^* \vec{\nabla}\psi - \vec{\nabla}\psi^* \psi\right)$$

Born approximation (Sakurai P 399 - 403)

under weak scattering $\rightarrow \langle r | \psi^+ \rangle \simeq \langle r | \phi \rangle = \exp(i\vec{k}\cdot\vec{r})/(2\pi)^{3/2}$

First (order) Born approximation ($V(\vec{k}-\vec{k}')$ fourier transformed potential)

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17. 10. 2018

Higher order Born Approximation

Optical theorem

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22. 10. 18

deriving optical theorem:

$$\operatorname{Im}\langle \vec{k} | \hat{T} | \vec{k} \rangle = \operatorname{Im}\langle \vec{k} | \hat{V} | \psi^+ \rangle$$

$$\operatorname{Im}\left(\overbrace{\left(\langle \psi^+ | - \langle \psi^+ | \hat{V} \frac{1}{E - \hat{H}_0 - i\varepsilon}\right)}\hat{V} | \psi^+ \rangle\right)$$

$$= \underbrace{\mathrm{Im}\langle\psi^+|\hat V|\psi^+\rangle}_{=0} - \sum_{k'} \langle\psi^+|\hat V|\vec k'\rangle \,\mathrm{Im}\left(\frac{1}{E_k - E_{k'} - i\varepsilon}\right) \langle\vec k'|\hat V|\psi^+\rangle$$

$$= \int d^3k' \,|\langle\psi^+|\hat V|\vec k'\rangle|^2 \pi\,\delta(E_k - E_{k'})$$

$$\left[\begin{array}{ll} \mathrm{Im}\left(\frac{1}{x - i\varepsilon}\right) = \frac{\varepsilon}{x^2+\varepsilon^2} & \int_{-\infty}^{\infty} \frac{\varepsilon}{x^2+\varepsilon^2} = \pi \int_{-\infty}^{\infty} \frac{1}{x^2+} \, dx \cdot \chi \\ \lim\left(\frac{1}{\pi}\mathrm{Im}\frac{1}{x-i\varepsilon}\right) = \delta(x) & = \varepsilon t \\ & \uparrow \\ & dx = \varepsilon\, dt \end{array}\right]$$

$$\left[\begin{array}{ll} E_k = \frac{\hbar^2 k^2}{2m} & |\vec k| = |\vec k'| \\ \rightarrow dE_k = \frac{\hbar^2}{2m} 2k\,dk & \end{array}\right]$$

$$\Rightarrow \mathrm{Im}\langle\vec k|\hat T|\vec k\rangle = -\pi \frac{mk}{\hbar^2} \int d\Omega_{k'} \,|\langle\vec k'|\hat T|\vec k\rangle|^2 \quad \Big| \cdot -\frac{1}{4\pi}\left(\frac{2m}{\hbar^2}\right)(2\pi)^2$$

$$\mathrm{Im}\Big(\underbrace{-\frac{1}{4\pi}\left(\frac{2m}{\hbar^2}\right)(2\pi)^3\langle\vec k|\hat T|\vec k'\rangle}_{f(\vec k, \vec k')}\Big) = \frac{1}{4\pi}\left(\frac{2m}{\hbar^2}\right)(2\pi)^3 \pi \frac{mk}{\hbar^2} \int d\Omega_{k'} \,|\langle\vec k'|\hat T|\vec k\rangle|^2$$

$$= \frac{\pi m k}{\hbar^2} \frac{4\pi}{(2\pi)^3}\left(\frac{\hbar^2}{2m}\right) \int d\Omega_{k'} \,|f(\vec k', \vec k)|^2$$

$$= \frac{k}{4\pi}\sigma_{tot}$$

Eikonal approximation: quasiclassical approximation

slowly varying potential $V(\vec r)$ $\quad \lambda\, |\partial_x V| << 1$

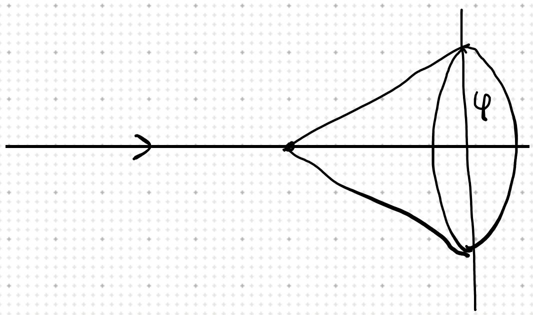
(Born approximation not applicable ?)

24.10.2018

- scattering Geometry in Eikonal approximation.
- Partial wave analysis

radial symmetric potential $\hat{V}(r) \rightarrow [\hat{H}, \hat{L}] = [\hat{H}, \hat{L}^2] = 0$

The expansion of scattering amplitude reduces to the $m=0$ component



$$\Rightarrow Y_\ell(\theta, \varphi) = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos\theta)$$

P_ℓ Legendre polynomials

The wave-function can be expanded as follows:

$$\psi_{out}(\vec{r}) = \sum_{\ell=0}^{\infty} \frac{u_\ell(r)}{r} P_\ell(\cos\theta)$$

The radial wave-function $u_\ell(r)$:

$$-\frac{\hbar^2}{2m} u_\ell''(r) + \left[V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right] u_\ell(r)$$

$$= E\, u_\ell(r)$$

(with radial potential it's always possible to reduce SE to 1d)

$$E = \frac{\hbar^2 k^2}{2m} \quad , \quad -\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\left(\partial_r^2 + \frac{2}{r}\partial_r\right) + \frac{\vec{L}^2}{2mr^2}$$

$$\Rightarrow \quad u'' + (k^2 - V_{eff}(r))\, u(r) = 0$$

if $V(r) = 0$, the solutions are plane waves!

Now the solutions which are regular at origin are the spherical Bessel-functions: $u_\ell(r) = i^\ell (2\ell+1) j_\ell(kr)$

For $r \gg R$: R. the range of the potential

$$u_\ell(r) \sim \frac{1}{k} i^\ell (2\ell+1) \sin(kr - \ell\pi/2) + \dots$$

For $V \neq 0$ we attempt to describe the wave-function with an ansatz:

$$u_l(r) = a_l \sin\left(kr - \frac{l\pi}{2} + \delta_l\right),$$

δ_l: scattering phase-shift of the l-th wave

The wave function $$\psi(\vec{r}) = \frac{e^{ikr}}{r} \sum_{l=0}^{\infty} \frac{a_l}{2i} e^{i\delta_l} e^{-il\pi/2} P_l(\cos\theta) + \frac{e^{-ikr}}{r} \sum_{l=0}^{\infty} \frac{a_l}{2i} e^{-i\delta_l} e^{il\pi/2} P_l(\cos\theta)$$

$$\psi(\vec{r}) = \left\{ \frac{e^{ikr}}{r} \left[\sum_l \frac{i^l}{2i} (2l+1) e^{-il\pi/2} P_l(\cos\theta) + f(\theta) \right] + \frac{e^{-ikr}}{r} \frac{1}{k} \frac{i^l}{2i} 2l\, e^{i\pi l/2} P_l(\cos\theta) \right] \right\}$$

$$\psi = e^{i\vec{k}\cdot\vec{r}} + f(\theta) \frac{e^{ikr}}{r}$$

29.10.2018

- Partial-Wave analysis of scattering: (in spherical potentials)

Sakurai P 409 – 413

Angular momentum

$$|\vec{L}| = |\vec{r} \times \vec{p}| = b\, p_\infty = b\sqrt{2mE}$$

The potential only "acts" if $b < R$

$L < R\sqrt{2mE}$ $\qquad l < R\sqrt{\frac{2mE}{\hbar^2}} = kR$ $\Rightarrow$ partial waves decay for $l \gg kR$

Elektron – silicon (foreign atoms) - scattering

s ($l=0$) - wave only $\qquad \frac{d\sigma}{d\Omega} \sim \frac{1}{k^2} \sin^2 \delta_0$

Sakurai P 414 – 417

Scattering from a hard sphere $\longrightarrow$ test, oral exam

05.11.2018 Sakurai 420 – 423, 424 – 428

- Scattering from the hard sphere

in the limit $kR \gg 1$ high energy limit

$$\sum_{0\le l<kR} (2l+1)\sin^2\delta_l \simeq \int_0^{kR} dl\ (2l+1)\sin^2(kR - l\pi/2)$$

$$\left(\tfrac{1}{2}kR\right)^2 + \tfrac{1}{2}(kR)\left(1+\tfrac{2}{\pi}\sin(kR(2-\pi))\right) + \mathcal{O}(1)$$

$$\Rightarrow \sigma_{tot} = 2\pi R^2\left(1+\mathcal{O}(1/kR)\right)$$

Scattering amplitude:

$$f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)e^{i\delta_l}\sin\delta_l P_l(\cos\theta)$$

$$= \underbrace{\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)e^{2i\delta_l}P_l(\cos\theta)}_{f_{reflection}} + \underbrace{\frac{i}{2k}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)}_{f_{shadow}}$$

Assumption: $kR \gg 1$, $\delta_l = 0$ for $l > kR$

Total cross section:

$$\sigma_{tot} = \int d\Omega\ |f_s(\theta)|^2 + \int d\Omega\ |f_R(\theta)|^2$$
$$+ 2\,\mathrm{Re}\int d\Omega\ f_s^*(\theta) f_R^*(\theta) \leftarrow \text{interference}$$

Discuss contributions separately:

1: $$\int d\Omega\ |f_R(\theta)|^2 = \frac{2\pi}{4k^2}\sum_{0\le l\le kR}(2l+1)^2\int d(\cos\theta)\,P_l^2(\cos\theta) = \frac{\pi}{k^2}\sum(2l+1)$$

$$= \pi R^2\left(1+\mathcal{O}\left(\tfrac{1}{kR}\right)\right)$$

2: Integral representation of $P_l(\cos\theta) = \frac{1}{\pi}\int_0^{\pi} d\varphi\,(\cos\theta + i\sin\theta\cos\varphi)^l$

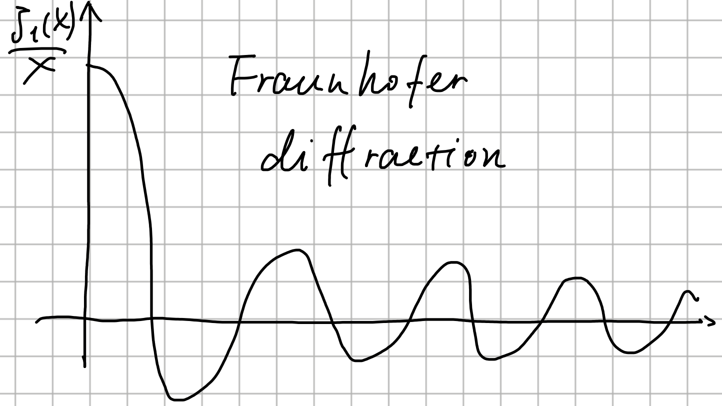
Harish-Chandra, Gelfand-Naimark, Laplace

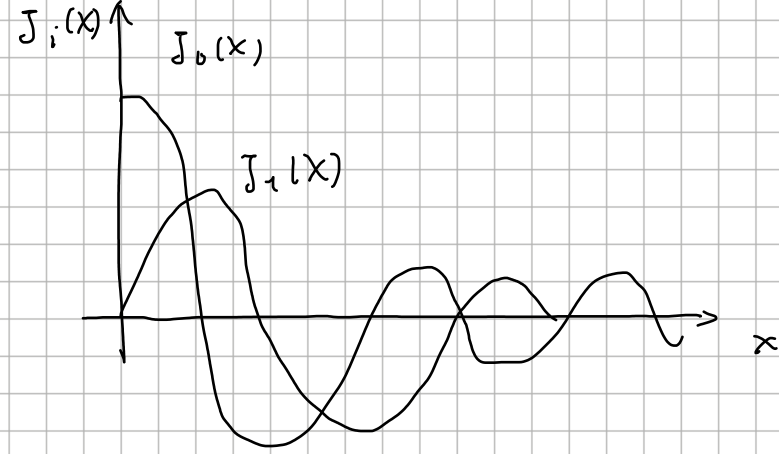
For large energies $\theta \ll 1$:

$$P_l(\cos\theta) = \frac{1}{\pi}\int_0^{\pi} d\varphi\ e^{l\log(\cos\theta + i\sin\theta\cos\varphi)}$$

$$\Rightarrow P_l(\cos\theta) = \frac{1}{\pi}\int_0^{\pi} d\varphi\ \exp(i\theta l\cos\varphi) = J_0(l\theta)\left(1+\mathcal{O}(\theta^2)\right)$$

$$\sum_{0\le l\le kR}(2l+1)J_0(l\theta) \simeq \int_0^{kR} dl\ (2l+1)J_0(l\theta) \simeq \frac{2(kR)^2 J_1(kR\theta)}{(kR\theta)}$$





$$\int d\Omega \, |f_s(\theta)|^2 = \frac{2\pi}{4k^2} \int_0^\pi d\theta \, (4kR) J_1^2(kR\theta) / \theta^2 \cdot \sin\theta$$

Main contribution of integral comes from $\theta = 0$

$$\simeq 2\pi R^2 \int_0^\pi d\theta \frac{J_1^2(kR\theta)}{\theta} = 2\pi R^2 \int_0^{\pi kR} dx \; \frac{J_1^2(x)}{x}$$

$$\simeq 2\pi R^2 \int_0^\infty dx \frac{J_1^2(x)}{x} = \pi R^2$$

$$\Rightarrow \int d\Omega \, |f_s(\theta)|^2 = \pi R(1 + \mathcal{O}(1/kR))$$

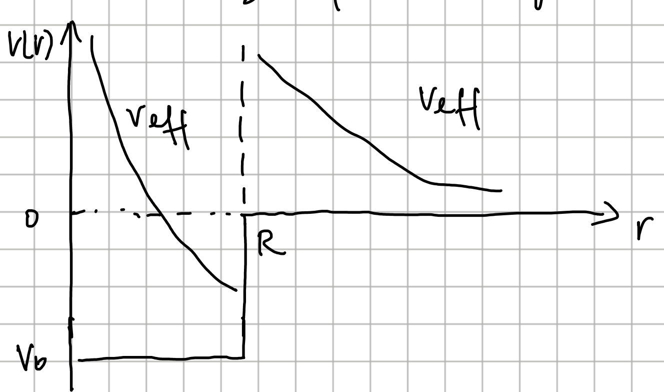
③: interference term $2\mathrm{Re}(f_R^* f_s)$

cancelation due to fluctuations

— Rectangular - barier:

7.11.2018

Scattering from a potential Wall



$$\frac{\hbar^2 k^2}{2m} = E \qquad \frac{\hbar^2 k'^2}{2m} = E - V_0$$

$$R_\ell \begin{cases} A_\ell \, j_\ell(k'r) & 0 \le r < R \\ a_\ell j_\ell(kr) + b_\ell n_\ell(kr) & r \ge R \end{cases}$$

→ Match logarithmic derivative at $r = R$

$$\left.\frac{1}{R_\ell} \frac{dR_\ell}{dr}\right|_{r=R} \text{ continuous} \Rightarrow k' \frac{j_\ell'(k'R)}{j_\ell(kR)} = k \frac{a_\ell j_\ell'(kR) + b_\ell n_\ell'(kR)}{a_\ell j_\ell(kR) + b_\ell n_\ell(kR)}$$

For $l=0$ $\qquad \delta_0 = \mathrm{arctg}\left(k/k' \,\mathrm{arctg}(k'R)\right) - kR$

$kR \ll 1$ $\qquad$ low energy scattering

$$\mathrm{tg}\,\delta_l = \frac{k\, j_l'(kR)\, j_l(k'R) - k'\, j_l(k'R)\, j_l(kR)}{k\, n_l'(kR)\, j_l(k'R) - k'\, j_l'(k'R)\, n_l(kR)}$$

Simplify for $kR \ll 1$:

$$\mathrm{tg}\,\delta_l = \underbrace{\frac{(2l+1)}{((2l+1)!!)^2}(kR)^{2l+1}}_{\ll 1,\ \text{small}} \; \underbrace{\frac{l\, j_l(k'R) - (kR)\, j_l'(k'R)}{(l+1)\, j_l(k'R) + k'\, j_l'(k'R)}}_{\text{can be zero!}}$$

$kR \ll 1$, $k'R \gg l$ $\qquad k' = \sqrt{2m(E_0 - V)}/\hbar$

$$j_l(k'R) \simeq \frac{1}{k'R}\sin(k'R - l\pi/2)$$

$$j_l'(k'R) \simeq -\frac{1}{(k'R)^2}\sin(k'R - l\pi/2) + \frac{1}{k'R}\cos(k'R - l\pi/2)$$

$\Rightarrow$ denominator of $\mathrm{tg}\,\delta_l$:

$$\left(\frac{(l+1)}{k'R} - \frac{k'R}{(k'R)^2}\right)\sin(k'R - l\pi/2) + \cos(k'R - l\pi/2) \overset{!}{=} 0$$

$$\frac{l}{k'R}\sin(k'R - l\pi/2) + \cos(k'R - l\pi/2) = 0$$

$$\mathrm{ctg}(k'R - l\pi/2) = -\frac{l}{k'R}$$

$\Rightarrow$ equation for k' or E $\longrightarrow$ Resonance E_{Res}

$$k'R - l\pi/2 \simeq (m + \tfrac{1}{2})\pi - l/k'R$$

Close to solution of resonance condition $\mathrm{tg}\,\delta_l$ diverges

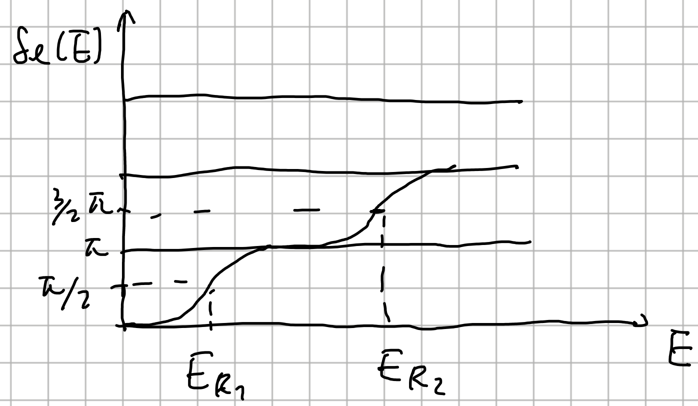
$$\Rightarrow \delta_l(E = E_R) = \frac{\pi}{2}(2m+1) \quad \text{for some } m \in \mathbb{Z}$$

Expand around $E = E_R$

$$\boxed{\mathrm{tg}\,\delta_l = \gamma_l \frac{(kR)^{2l+1}}{E - E_R}}$$

$$\gamma_l = \frac{2l+1}{((2l+1)!!)^2} \left.\frac{l\, j_l(k'R) - k'R\, j_l'(k'R)}{\frac{d}{dE}\left((l+1)\, j_l(k'R) + k'R\, j_l(k'R)\right)}\right|_{E=E_R}$$

Behaviour of δ_ℓ as a function of energy:



Total cross section of partial wave ℓ:

$$\sigma_\ell = \frac{4\pi(2\ell+1)}{k^2} \sin^2\delta_\ell = \frac{4\pi(2\ell+1)}{k^2} \frac{tg^2\delta_\ell}{1+tg^2\delta_\ell}$$

$$\Rightarrow \sigma_\ell = \underbrace{\frac{4\pi(2\ell+1)}{k^2}}_{\sigma_{max}} \frac{\gamma_\ell^2 (kR)^{4\ell+2}}{1+\gamma_\ell^2(kR)^{4\ell+2}}$$

Breit - Wigner - Equation

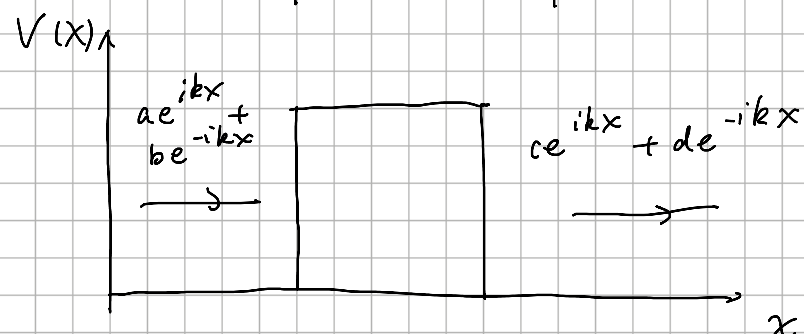
$$\Delta E_\ell = 2|\gamma_\ell|(kR)^{2\ell+1}$$

12.11.2018

Analytic properties of the scattering

Scattering in 1D

$$|\psi_{out}\rangle = \hat{S}\,|\psi_{in}\rangle$$



$$|\psi_{in}\rangle = ae^{ikx} + de^{-ikx}$$
$$|\psi_{out}\rangle = ce^{ikx} + be^{-ikx}$$

$$\Rightarrow \begin{pmatrix} b \\ c \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} \begin{pmatrix} a \\ d \end{pmatrix}$$

For $V(x)$ real we have

time reversal $\longrightarrow$ $|\psi_{in}\rangle^* = \hat{S}\,|\psi_{out}\rangle^*$ $\Rightarrow$ $\hat{S}^* = \hat{S}^{-1}$ unitary!

$\Rightarrow$ The scattering amplitude for the partial wave l defined by $S_l(k) = 1 + 2ik f_l(x)$ $\Rightarrow$ $|S_l(k)| = 1$ is the diagonal matrix element of $\hat{S}$ matrix in the l potential

Bound state

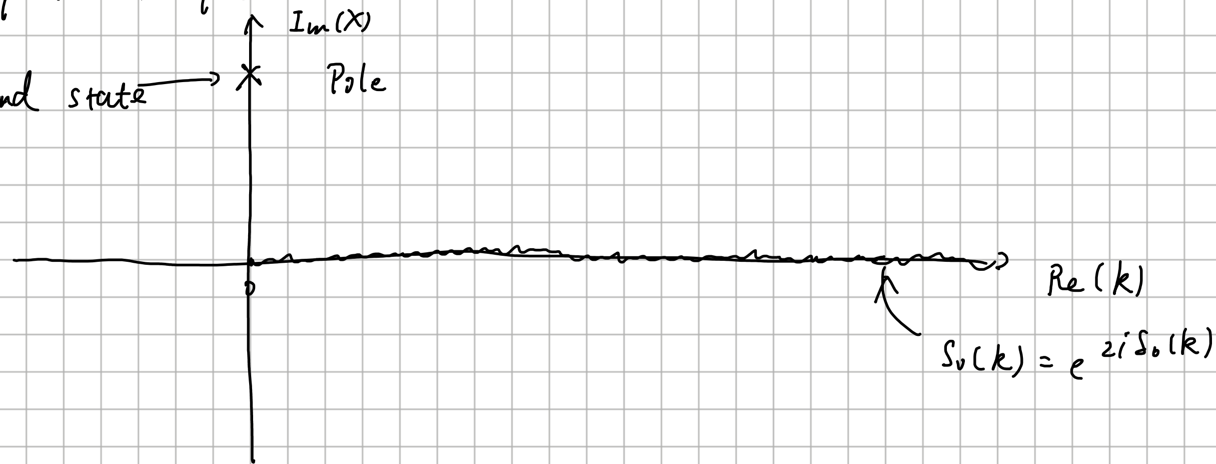
$l = 0$. The radial wave function takes the form

$$\sim S_0(k)\,\frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}$$

The asymptotic form of a bound state: $e^{-\varkappa r}/r$

normalization $\longrightarrow$ $\sim e^{-\varkappa r}/r - \dfrac{1}{S_0(k)}\dfrac{e^{\varkappa r}}{r}$ if $S_0(\varkappa) \to \infty$

Complex k-plane:

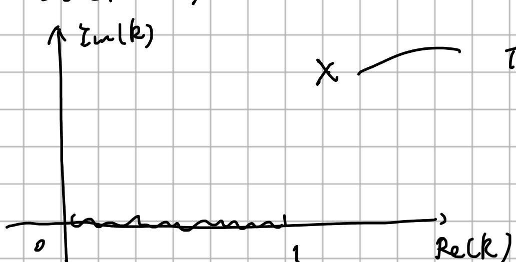


$$f(x+iy) = u(x,y) + i\,V(x,y)$$

$(\partial_x^2 + \partial_y^2)\,u(x,y) = 0$ $\iff$ $f(x+iy)$ is analytic

$(\partial_x^2 + \partial_y^2)\,V(x,y) = 0$

- Poles at bound state at $Re(k) = 0$ on the imaginary axis
- $|S_0(x)| = 1$ for all k with $Re(k) > 0$. $Im(k) = 0$.
- $S_0(k=0) = 1$



The $S_0(k)$ here: $f(z) = \dfrac{1}{2\pi}\int_0^1 dx\,\dfrac{1}{z-x}$