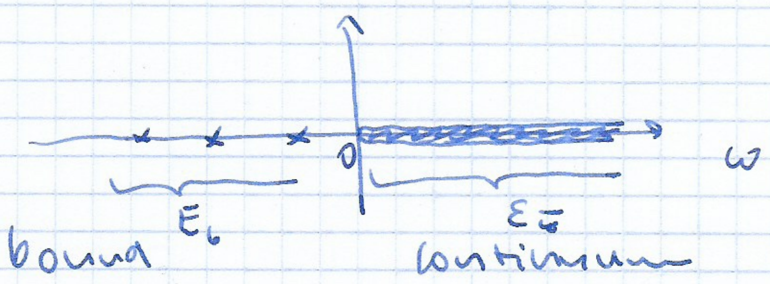
• Bound and continuum states

Levinson theorem

$$\hat{G}(z) = \sum_b \frac{|\psi_b\rangle\langle\psi_b|}{z - E_b} + \int d_3k \frac{|\vec{k}\rangle\langle\vec{k}|}{z - \varepsilon_{\vec{k}}}$$



$$\sum_b |\psi_b\rangle\langle\psi_b| + \int d_3k\, |\vec{k}\rangle\langle\vec{k}| = \mathbb{1}$$

The change in DOS at ω

$$\Delta\rho(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \frac{\partial}{\partial z} \operatorname{Im} \operatorname{Tr}\left[\ln\left(1 - \hat{G}_0(z)\hat{V}\right)\right]$$

note

$$\operatorname{Tr}\left[\ln\left(1 - \hat{G}_0(z)\hat{V}\right)\right] =$$

$$= \sum_i \ln\left(1 - \hat{G}_0(z)\hat{V}\right)_{ii} =$$

$$= \ln \prod_i \left(1 - \hat{G}_0(z)\hat{V}\right)_{ii} =$$

$$= \ln \operatorname{Det}\left(\mathbb{1} - \hat{G}_0(z)\hat{V}\right) = \ln D(z)$$

Df Fredholm determinant

$$\boxed{D(z) = \operatorname{Det}\left(\mathbb{1} - \hat{G}_0(z)\hat{V}\right)}$$

$$\boxed{\Delta\rho(\omega) = -\frac{1}{\pi} \lim_{\eta \to 0^+} \frac{\partial}{\partial z} \operatorname{Arg}\left(D(z)\right)}$$

also $\boxed{\operatorname{Tr} \hat{\delta}(z) = -\operatorname{Arg} D(z)}$

For a bound state $\omega = E_b$

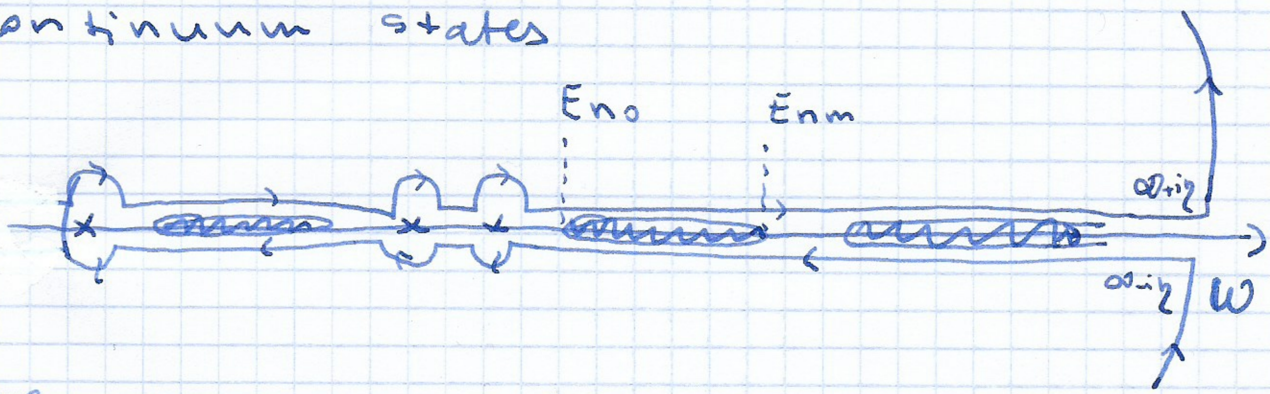
$$-\frac{1}{\pi} \, \mathrm{Im} \frac{d}{dz} \ln(z - E_b) \xrightarrow[\eta \to 0]{} \delta(\omega - E_b)$$

$$\int_{-\infty}^{0} \Delta\rho(\omega)\, d\omega = \int_{-\infty}^{0} \sum_b \delta(\omega - E_b)\, d\omega = N_b$$

[number of bound states]

$\square$

Consider a situation where we have N_b bound states and some number of continuum states



Theorem

$$\frac{1}{2\pi i} \oint_C \underbrace{\frac{f'(z)}{f(z)}}_{(\ln f(z))'} dz = N - P$$

if $f(z)$ analytic in and on C, apart of finite number of poles, and non-zero on C

N: number of zeros in contour C (a zero of m order is counted m times)

P: number of poles in C (a pole of order m is counted m times)

Compute $\frac{1}{2\pi i} \oint_C \ln D(z)' \, dz = ?$

i) contributions from bound states

$$(i) = -N_b$$

ii) contributions along $\mathbb{R}$

$$(ii) = \frac{1}{2\pi i} \underset{\substack{n \\ \uparrow \\ \text{band index}}}{\sum} \left\{ \ln \frac{D(E_{nm}^{+})}{D(E_{n0}^{+})} - \ln \frac{D(E_{nm}^{-})}{D(E_{n0}^{-})} \right\}$$

$$\boxed{D(E) = |D(E)| e^{i\delta(E)}}$$

Since $\quad \mathrm{Tr}\, \hat{\delta} = -\arg D(E^{+})$

$$(ii) = \frac{1}{\pi} \sum_n \mathrm{Tr} \left\{ \hat{\delta}(E_{n0}) - \hat{\delta}(E_{nm}) \right\}$$

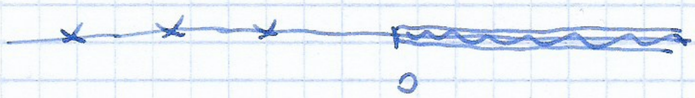
(ii) At ∞ $\quad \lim_{|\omega| \to \infty} D(\omega) = 1$ - finite on C_∞

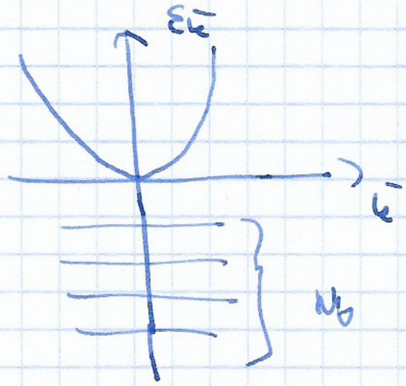
Hence

$$\boxed{\sum_n \mathrm{Tr} \left\{ \hat{\delta}(E_{n0}) - \hat{\delta}(E_{nm}) \right\} = N_b \cdot \pi}$$

<u>Levinson theorem</u>

For free electrons (one band $(0, \infty)$)





$$\mathrm{Tr} \left\{ \hat{\delta}(0) - \hat{\delta}(\infty) \right\} = N_b \pi$$

but $\quad \hat{\delta}(\infty) = 0$

$$\boxed{\mathrm{Tr}\, \hat{\delta}(0) = N_b \pi}$$

Fredholm determinants + Levinson theorem $\to$

$\to$ resonance states discussion

§7. SCATTERING AMPLITUDE

Lippmann-Schwinger equation for the wave function

$$\psi(\bar{r}) = \phi(\bar{r}) + \int d_3 r' \, G_0^+(\bar{r}, \bar{r}'; E) \, V(\bar{r}') \, \psi(\bar{r}')$$

where

$$G(\bar{r}, \bar{r}'; E) = -\frac{m}{2\pi\hbar^2} \frac{e^{ik|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|}$$

with

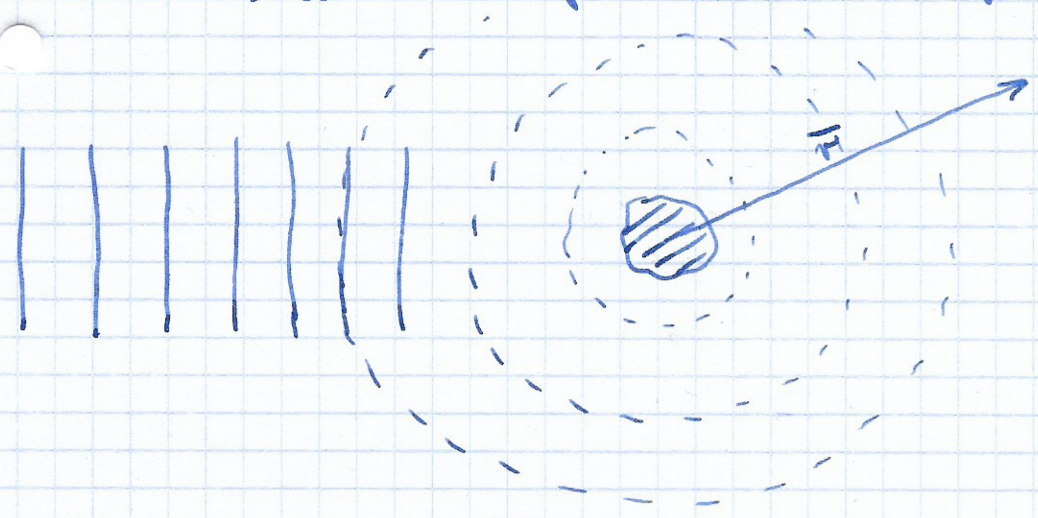
$$E = \frac{\hbar^2 k^2}{2m} \rightarrow k = k(E) = \sqrt{\frac{2mE}{\hbar^2}}$$

Solving L-S eq. iteratively we get the solution in terms of T-matrix

$$\boxed{\psi(\bar{r}) = \phi(\bar{r}) + \int d_3\bar{r}' \int d_3 r'' \, G_0(\bar{r}, \bar{r}'; E) \, T(\bar{r}', \bar{r}''; E) \, \phi(\bar{r}'')}$$

We analyze this solution at $r \to \infty$ limit

We assume a plane wave for the incident state



$$\phi(\bar{r}) = e^{i\bar{k}\cdot\bar{r}}$$

What is $\psi(\bar{r})$ at $|\bar{r}| \to \infty$?

$$\lim_{r\to\infty} \psi(\bar{r}) = e^{i\bar{k}\cdot\bar{r}} - \frac{m}{2\pi\hbar^2} \lim_{r\to\infty} \int d_3 r \int d_3 r' \cdot$$

$$\cdot \frac{e^{ik|\bar{r}-\bar{r}'|}}{|\bar{r}-\bar{r}'|} T(\bar{r}', \bar{r}'') e^{i\bar{k}\cdot\bar{r}''}$$

$$\bar{r} = r\hat{e}_r(\theta, \varphi) = r(\cos\theta\, \hat{e}_z + \sin\theta\cos\varphi\, \hat{e}_x + \sin\theta\sin\varphi\, \hat{e}_y)$$

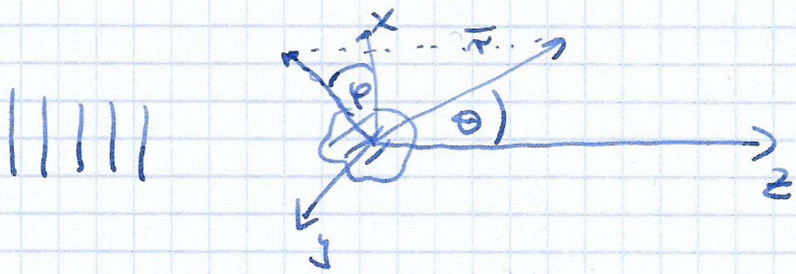
$$|\bar{r} - \bar{r}'| = \sqrt{(\bar{r} - \bar{r}')^2} =$$

$$= \sqrt{r^2 - 2r\hat{e}_r\cdot\bar{r}' + r'^2} =$$

$$= r\sqrt{1 - 2\frac{\hat{e}_r\cdot\bar{r}'}{r} + \left(\frac{r'}{r}\right)^2} \underset{r \gg r'}{\simeq}$$

$$\simeq r\left(1 - \frac{\hat{e}_r\cdot\bar{r}'}{r}\right) = r - \hat{e}_r\cdot\bar{r}'$$

We choose $\hat{e}_z$ along $\bar{k}$ so that $\theta = 0$ corresponds to the forward scattering direction



Also $\lim_{r\to\infty} \frac{1}{|\bar{r}-\bar{r}'|} \simeq \frac{1}{r}$

Hence,

$$\lim_{r\to\infty} G_0^+(\bar{r}, \bar{r}') = -\frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} e^{-ik\hat{e}_r\cdot\bar{r}'}$$

At large r

$$\psi(\vec{r}) = e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d_3r'\int d_3r''\, e^{-ik\hat{e}_r\cdot\vec{r}'}\, T(\vec{r}',\vec{r}'')\, e^{ikz''}$$

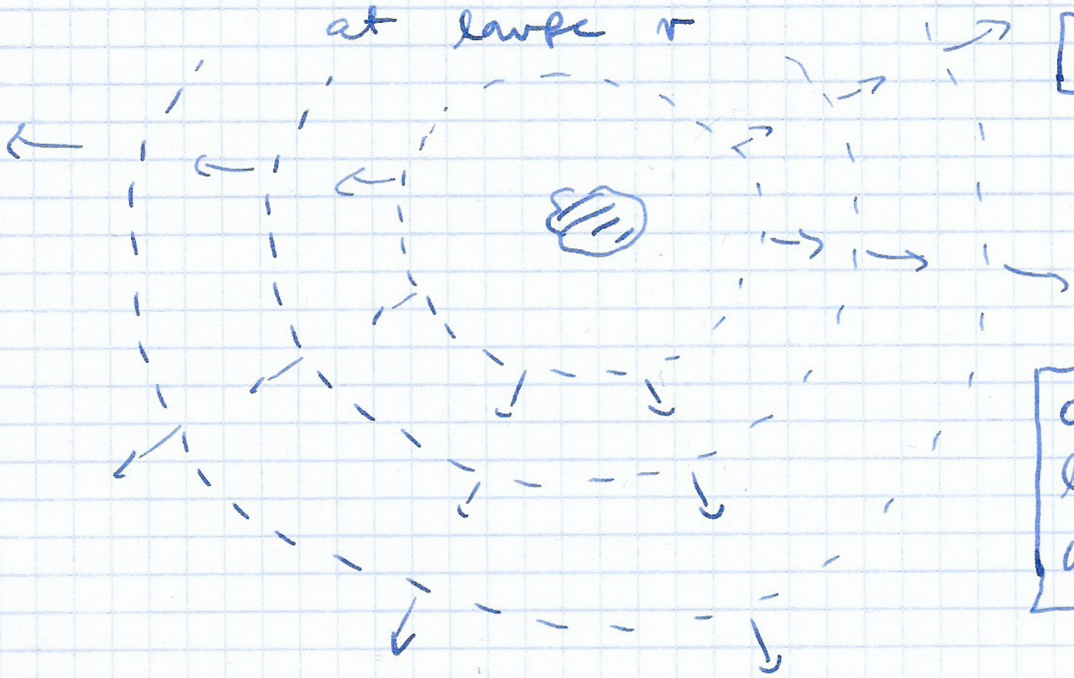
Df. <u>Scattering amplitude</u> $f_k(\theta,\varphi)$

$$\boxed{\lim_{r\to\infty}\psi(\vec{r}) = e^{ikz} + f_k(\theta,\varphi)\frac{e^{ikr}}{r}}$$

Hence,

$$\boxed{f_k(\theta,\varphi) = -\frac{m}{2\pi\hbar^2}\int d_3r'\int d_3r''\, e^{-ik\hat{e}_r\cdot\vec{r}'}\, T(\vec{r}',\vec{r}'')\, e^{ik\hat{e}_z\cdot\vec{r}''}}$$

Remark: The $E \to E + i0^+$ trick, equivalent to retarded boundary condition G^+ yields outgoing spherical wave at large r



$$\boxed{E \to E + i0^+}$$
$$\Updownarrow$$
$$\boxed{\theta(t-t')}$$
$$\Updownarrow$$
$$\boxed{\text{outgoing boundary condition}}$$

Mathematically $E \to E - i0^+$ which would lead to advanced boundary condition or incoming b.c.

$$\boxed{E \to E - i0^+}$$

$$\Updownarrow$$

$$\boxed{\theta(t'-t)}$$

$$\Updownarrow$$

incoming boundary condition

$$f = \frac{e^{-ikr}}{r}$$

$\square$

With the substitution

$$k\hat{e}_r \to \bar{k}' \qquad (k = k' \text{ in elastic scatt.})$$

$$k\hat{e}_z \to \bar{k}$$

$$\boxed{f(\bar{k}, \bar{k}')} = -\frac{m}{2\pi\hbar^2} \int d_3r' \int d_3r'' e^{-i\bar{k}'\cdot\bar{r}'} T(\bar{r}', \bar{r}'') e^{i\bar{k}\cdot\bar{r}''} =$$

$$= -\frac{(2\pi)^2 m}{\hbar^2} \int d_3r' \int d_3r'' \langle \bar{k}' | \bar{r}' \rangle \langle \bar{r}' | \hat{T} | \bar{r}'' \rangle \langle \bar{r}'' | \bar{k} \rangle$$

$$\boxed{= -\frac{(2\pi)^2 m}{\hbar^2} \langle \bar{k}' | \hat{T} | \bar{k} \rangle}$$

transition amplitude between incident wave $|\bar{k}\rangle$ and outgoing wave $|\bar{k}'\rangle$

$f(\bar{k}, \bar{k}')$ – valid also in inelastic scattering (not discussed here)

scattering amplitude $\simeq$ Fourier transform of the T-matrix

Scattering cross section

$$dN = \vec{j}_{scatt} \cdot d\bar{S} = r^2 \vec{j}_{scatt}\, \hat{e}_r\, d\Omega =: j_{inc} \cdot d\sigma$$

$$\phi(\bar{r}) = e^{ikz} \quad \to \quad j_{inc} = \frac{\hbar k}{m}$$

$$\psi(r) \sim f_k(\theta, \varphi) \frac{e^{ikr}}{r}$$

$$\vec{j}_{scatt} \cdot \hat{e}_r = j_{scatt,\, r} = \frac{\hbar}{2mi}\left(\psi^*_{scatt} \frac{\partial}{\partial r} \psi_{scatt} - \psi_{scatt} \frac{\partial}{\partial r} \psi^*_{scatt} \right) =$$

$$= \frac{\hbar k}{m} \frac{1}{r^2} |f_k(\theta, \varphi)|^2$$

$$\Rightarrow \quad \boxed{\frac{d\sigma}{d\Omega} = |f(\bar{k}, \bar{k}')|^2}$$

or

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{(2\pi)^4 m^2}{\hbar^4} |\langle \bar{k}' | \hat{T} | \bar{k} \rangle|^2}$$

Different formulation of the optical theorem

$$\operatorname{Im} f(\bar{k}, \bar{k}) = -\frac{(2\pi)^2 m}{\hbar^2} \operatorname{Im} T_{\bar{k}\bar{k}}(E) =$$

forward $\theta = 0$ scattering amplitude

$$= -\frac{(2\pi)^2 m}{\hbar^2} \frac{1}{2i}\left(T_{\bar{k}\bar{k}}(E) - T^*_{\bar{k}\bar{k}}(E) \right) =$$

$=$ optical theorem (page 110) $=$

$$= \frac{(2\pi)^2 m}{\hbar^2} \pi \int d\Omega_p \int dp\, p^2 \, |T_{kp}|^2 \, \delta\left(E - \frac{\hbar^2 p^2}{2m}\right) =$$

$$= \frac{1}{4\pi} \frac{2mE}{\hbar^2} \int d\Omega \, \frac{d\sigma}{d\Omega} =$$

$$\delta(f(x)) = \frac{\delta(x - x_0)}{|f'(x_0)|}$$

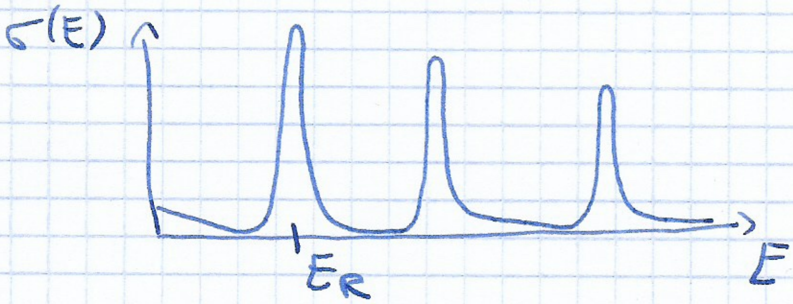
$$= \frac{k}{4\pi} \sigma$$

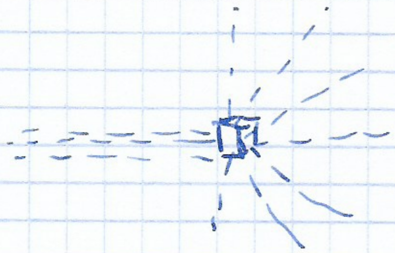
$$\boxed{\operatorname{Im} f(\bar{k}, \bar{k}') = \operatorname{Im} f(\theta = 0) = \frac{k}{4\pi} \sigma(E)}$$

Exact sum rule → self-consistency check.

§8. RESONANCE STATES

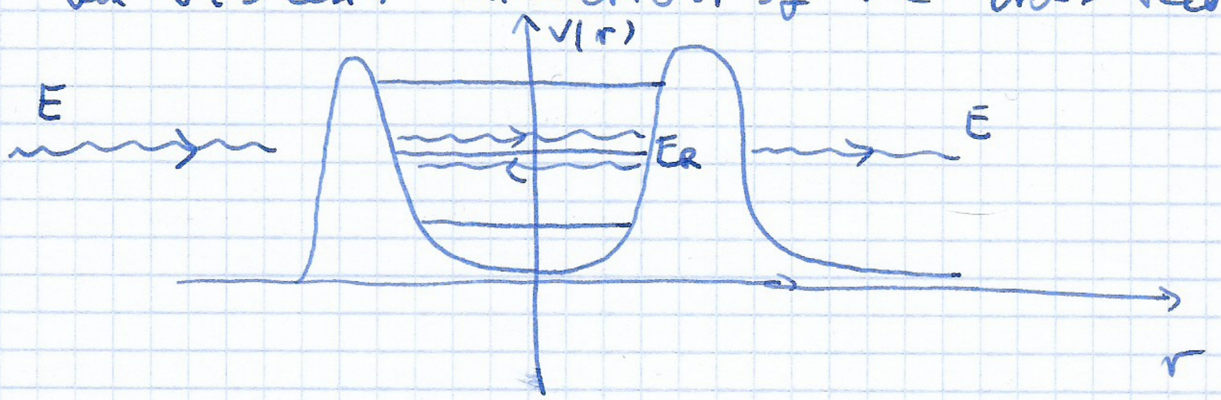
some experiments show a sharp peak(s) in total cross section





They are associated with "nearly bound states" in the scattering potential at E_R

When incident particles hit the scattering potential / target with having energy E_R they are temporarily captured in to this "metastable" state giving rise to a ~~va~~ violent variation of the cross section



$$E \simeq E_R \quad \text{resonance condition}$$

Such states are named ~~to~~ <u>resonance states</u>.

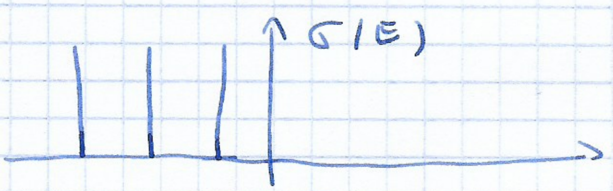
How to describe such states?

$$\sigma(E) = \frac{4\pi}{k}\, \mathrm{Im}\, f(\bar{k},\bar{k}) = -\left(\frac{2}{k}\right)\frac{(2\pi)^3 m}{\hbar^2}\, \mathrm{Im}\, \langle \bar{k}|\hat{T}|\bar{k}\rangle$$

$$\hat{T}(E) = \frac{\hat{V}}{1-\hat{G}_0(E)\hat{V}}$$

Note: If $\langle \bar{k}|1-\hat{G}_0(E)\,\hat{V}|\bar{k}\rangle\Big|_{E=E_b} = 0$ then $T_{\bar{k}\bar{k}}(E_b) \to \infty$

↑ pole of $\hat{T}(E)$



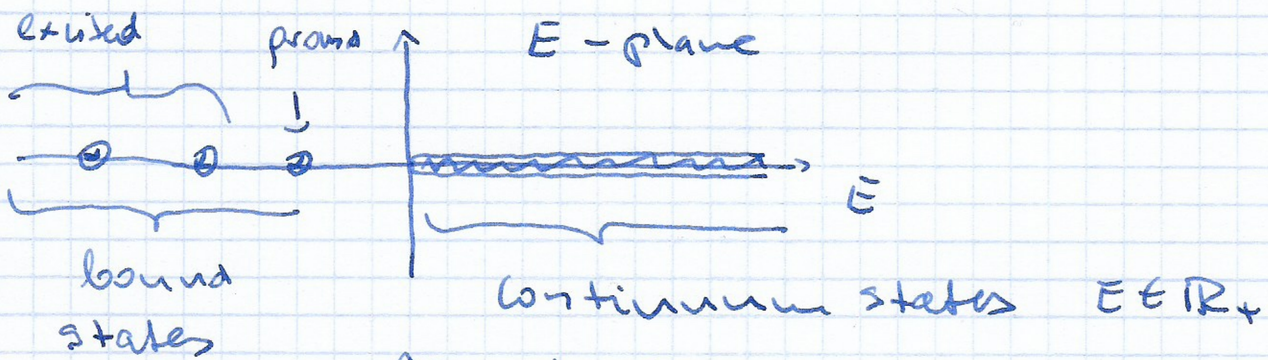
(i) The system has a <u>bound states</u>: poles at

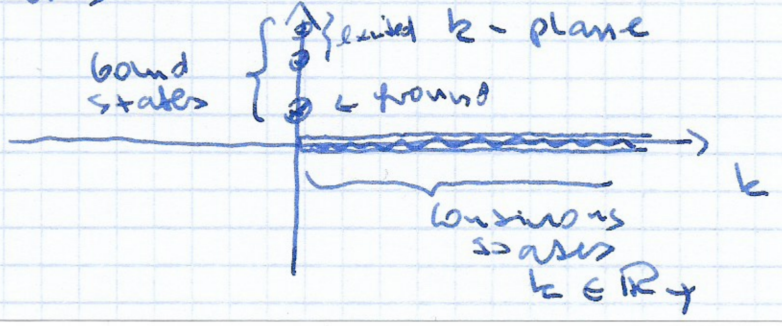
real energies $E = E_b = -\dfrac{\hbar^2 \varkappa_b^2}{2m}$

and $k = i\varkappa_b$, $\underline{\varkappa_b > 0}$

The bound state wave function

$$\Psi_b(r,t) \sim \frac{e^{-\varkappa_b r}}{r} \cdot e^{-i\frac{E_b t}{\hbar}}$$





(ii) Formally, there are also <u>virtual states</u>

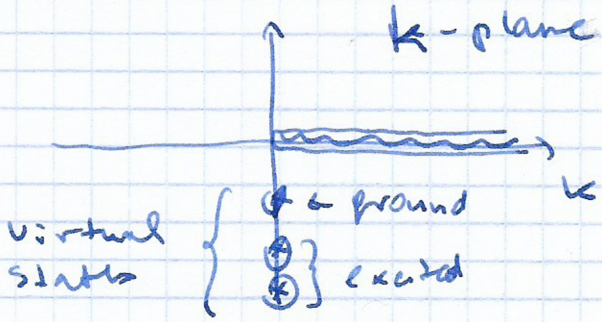
poles at real energies

$$E = E_v = -\frac{\hbar^2 \varkappa_v^2}{2m}$$

and $k = i\varkappa_v$, $\underline{\underline{\varkappa_v < 0}}$

the wave function

$$\Psi_v(r,t) \sim \frac{e^{|\varkappa_v| r - i\frac{E_v t}{\hbar}}}{r}$$ – <u>not normalized!</u>

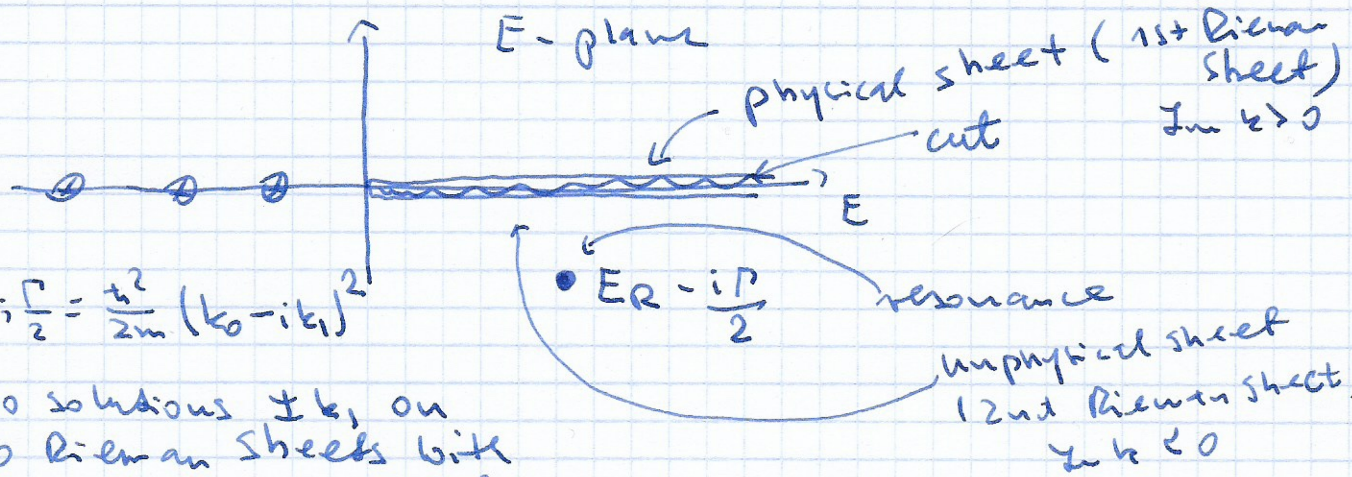


(iii) <u>resonance states</u>

poles of $T(E)$ at complex E

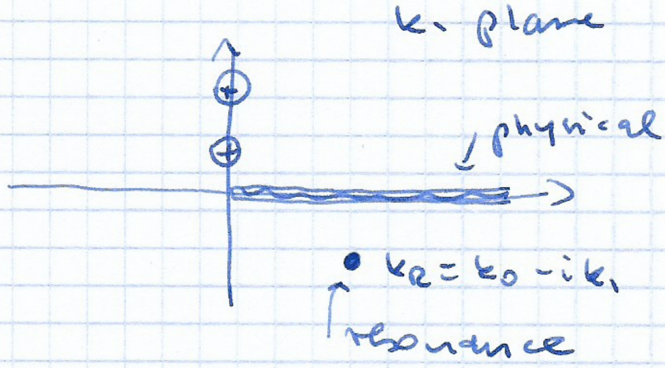
$$E = E_R - i\frac{\Gamma}{2}$$

and $k_R = k_0 - ik_1$ $\qquad k_0, k_1 \in \mathbb{R}$



$$E_R - i\frac{\Gamma}{2} = \frac{\hbar^2}{2m}(k_0 - ik_1)^2$$

two solutions $\pm k_1$ on two Rieman Sheets with the same value of $E = \frac{\hbar^2 k^2}{2m}$



the wave function

$$\boxed{\psi_R(r) \sim \frac{e^{ikr}}{r} = \frac{e^{ik_0 r}}{r}\, e^{k_1 r}}$$

ascending outgoing wave
(unstable bound state)

proof $$k = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2mE_R}{\hbar^2} - i\,\frac{m\Gamma}{\hbar^2}} =$$

$\Gamma \ll E_R$

$$= \sqrt{\frac{2mE_R}{\hbar^2}}\,\sqrt{1 - i\,\frac{\Gamma}{2E_R}} \simeq$$

$$\simeq \underbrace{\sqrt{\frac{2mE_R}{\hbar^2}}}_{k_0} - i\,\underbrace{\sqrt{\frac{2mE_R}{\hbar^2}}\,\frac{\Gamma}{2E_R}}_{k_0} = k_0 - ik_1$$

$\square$

$$\psi_R(t) \sim e^{-i\frac{Et}{\hbar}} = e^{-i\frac{E_R t}{\hbar}}\, e^{-\frac{1}{2}\frac{\Gamma t}{\hbar}}$$

$$\boxed{|\psi_R(t)|^2 \sim e^{-\frac{\Gamma t}{\hbar}}} \qquad \boxed{\tau := \frac{\hbar}{\Gamma}}$$

lifetime of the resonance state

a state decaying in time

Breit-Wigners formula

Expand $\sigma(E)$ close to $E_R - i\frac{\Gamma}{2}$ for $\Gamma \ll E_R$

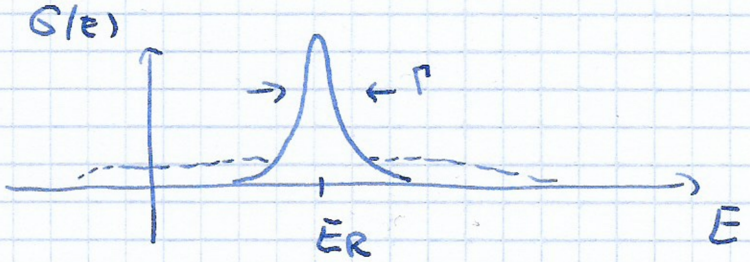
$$T_{kk}(E) \sim \frac{1}{E - E_R + i\frac{\Gamma}{2}}$$

$$\operatorname{Im} T_{kk}(E) \sim -\frac{\Gamma/2}{(E-E_R)^2 + (\frac{\Gamma}{2})^2}$$

Therefore

$$\boxed{\sigma(E) \simeq \sigma_0 \frac{\Gamma/2}{(E-E_R)^2 + (\frac{\Gamma}{2})^2}}$$

Lorentz shape function



How complex eigenvalues are possible?

Our system Hamiltonian is hermitian (elastic scattering, energy conserved)

$$\hat{H} = \frac{\bar{p}^2}{2m} + V(\bar{r}) = \left(\frac{\bar{p}^2}{2m}\right)^+ + V(\bar{r})^+ = \hat{H}^+$$

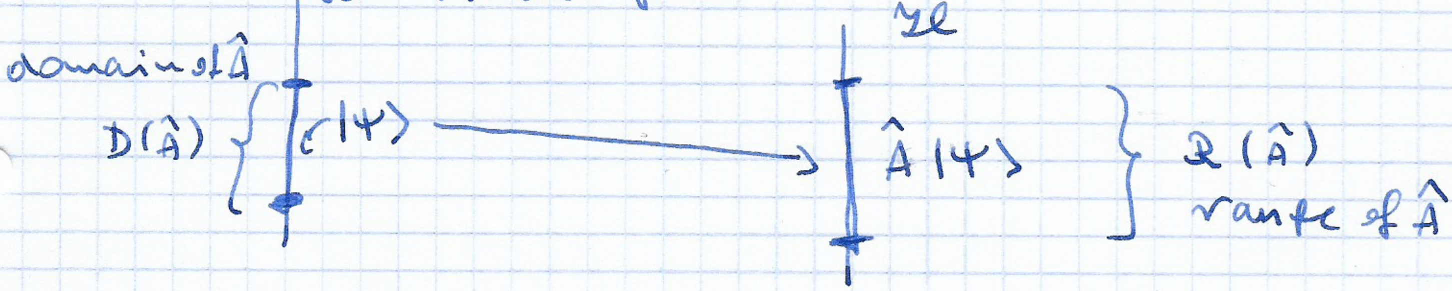
$\uparrow \mathbb{R}$ $\quad\quad$ $\uparrow \mathbb{R}$

$$\bar{p}^+ = \bar{p}$$

But: The eigenvalues of an operator $\hat{A}$ are real if the operator $\hat{A}$ is self-adjoint (hermitian $\hat{A}^+ = \hat{A}$ with the same domain $D(\hat{A}) = D(\hat{A}^+)$)

(i) $\boxed{\hat{A} = \hat{A}^+ \text{ – hermitian}}$

$\mathcal{H}$ – Hilbert space



(ii) $\boxed{D(\hat{A}) = D(\hat{A}^+)}$

By selecting the outgoing boundary condition $E + i0^+$

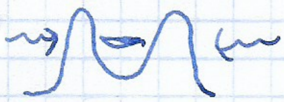
$\theta(t - t')$

$f \frac{e^{ikr}}{r}$ for Hamiltonians

the problem is not self-adjoint any more.

The domain of $\hat{H}^+$ is different and represented by ingoing boundary condition

$E - i0^+$



$\theta(t' - t)$

$f \frac{e^{-ikr}}{r}$ $\Rightarrow$ $\boxed{E \in \mathbb{C}}$

Resonant states are physical ones with complex eigenvalues. The choice of boundary condition matters → arrow of time

→ non-Hermitian quantum mechanics

→ ∃ Gamov vectors $|z_R\rangle$

→ Rigged Hilbert spaces (Maurin - Gelfand)