§5. FORMAL SOLUTION OF LIPPMAN-SCHWINGER EQUATION

The scattered state $|\psi_s\rangle = |\psi\rangle - |\phi\rangle$

L-S-Eq.

$$|\psi\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\psi\rangle$$

solve recursively

$$|\psi^0\rangle = |\phi\rangle$$

$$|\psi^1\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\phi\rangle$$

$$|\psi^2\rangle = |\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,|\phi\rangle + \hat{G}_0^+(E)\,\hat{V}\,\hat{G}_0^+(E)\,\hat{V}\,|\phi\rangle$$

$$\vdots$$

$$\boxed{|\psi\rangle = |\phi\rangle + \sum_{n=1}^{\infty}\left(\hat{G}_0^+(E)\,\hat{V}\right)^n|\phi\rangle}$$

It is like a geometric series which "converges" to

$$\boxed{|\psi\rangle = \frac{1}{1-\hat{G}_0(E)\,\hat{V}}\,|\phi\rangle}$$

$$(1-A)^{-1} = 1 + A + A^2 + \dots$$

For the scattered state

$$|\psi_s\rangle = \hat{G}_0^+\,\hat{V}\,|\phi\rangle + (\hat{G}_0^+\hat{V})^2\,|\phi\rangle + \dots =$$

$$= \hat{G}_0\,\hat{V}\,(1 + \hat{G}_0\,\hat{V} + (\hat{G}_0\,\hat{V})^2 + \dots)\,|\phi\rangle =$$

$$= \hat{G}_0\,\hat{V}\,(1-\hat{G}_0\,\hat{V})^{-1}\,|\phi\rangle$$

We introduce <u>T-matrix</u>

$$\boxed{\hat{T}(E) \equiv \hat{V}\left(1 - \hat{G}_0^+(E)\hat{V}\right)^{-1}}$$

or equivalently $\boxed{\hat{T}(E) = \left(1 - \hat{V}\hat{G}_0(E)\right)^{-1}\hat{V}}$

Indeed, by multiplying by $(1 - V\hat{G}_0^+)$ from the left and by $(1 - \hat{G}_0^+\hat{V})$ from the right

$$1)\quad (1 - \hat{V}\hat{G}_0^+)\hat{T}(1 - \hat{G}_0^+\hat{V}) = (1 - \hat{V}\hat{G}_0^+)\hat{V}\overbrace{(1 - \hat{G}_0^+\hat{V})^{-1}(1 - \hat{G}_0^+\hat{V})}^{1}$$

$$\|$$

$$2)\quad (1 - \hat{V}\hat{G}_0^+)\hat{T}(1 - \hat{G}_0^+\hat{V}) = \underbrace{(1 - \hat{V}\hat{G}_0)(1 - \hat{V}\hat{G}_0)^{-1}}_{1}\hat{V}(1 - \hat{G}_0\hat{V})$$

$$\rightarrow \quad \hat{V} - \hat{V}\hat{G}_0^+\hat{V} = \hat{V} - \hat{V}\hat{G}_0^+\hat{V}$$

$\square$

<u>Expanding T-matrix</u>

$$\boxed{\hat{T}(E) = \hat{V} + \hat{V}\hat{G}_0^+(E)\hat{V} + \hat{V}\hat{G}_0^+(E)\hat{V}\hat{G}_0^+(E)\hat{V} + \dots}$$

T-matrix represents a series of multiple scatterings on potential $\hat{V}$

$$\boxed{|\psi_s\rangle = \hat{G}_0(E)\,\hat{T}(E)\,|\phi\rangle}$$

effective "scattering potential"

L-P equation for the wave function

$$\psi(r) = \langle r | \psi \rangle \quad , \quad \phi(r) = \langle r | \phi \rangle$$

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

where we used

$$\mathbb{1} = \int dr' \, |r'\rangle\langle r'|$$

and

$$\boxed{G_0^+(r, r'; E) = \langle r | \hat{G}_0^+(E) | r' \rangle}$$

is the Green's function

propagator from $|r'\rangle$ to $|r\rangle$

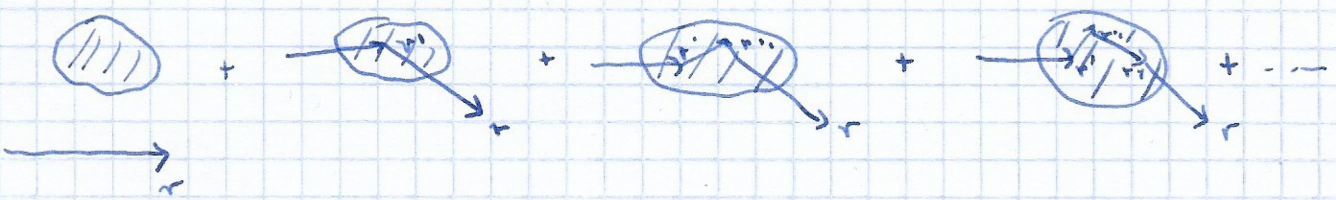
In terms of the infinite series

$$\boxed{\begin{aligned}\psi(r) = \phi(r) &+ \int dr' \, G_0^+(r, r'; E) \, V(r') \, \phi(r') + \\ &+ \int dr' \int dr'' \, G_0^+(r, r'; E) \, V(r') \, G(r', r'', E) \, V(r'') \, \phi(r'') + \\ &+ \cdots\end{aligned}}$$

Born series

$$\boxed{\begin{aligned}T(r, r', E) &= V(r) \, \delta(r - r') + V(r) \, G_0^+(r, r', E) \, V(r') + \\ &+ \int dr'' \, V(r) \, G_0^+(r, r', E) \, V(r') \, G_0^+(r', r'', E) \, V(r'') + \cdots\end{aligned}}$$

$$\boxed{T(r, r'; E) = \langle r | \hat{T}^+(E) | r' \rangle}$$



§6. FORMAL SOLUTION OF THE SCATTERING PROBLEM IN TERMS OF GREEN'S FUNCTIONS

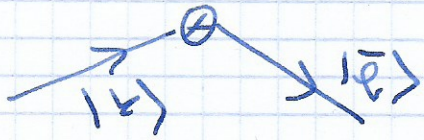
no bound states yet

$$\hat{H} = \hat{H}_0 + \hat{V} \qquad \varepsilon_{\bar{k}} \in \mathbb{R}$$

$$\hat{H}_0 = \sum_{\bar{k}} \varepsilon_{\bar{k}} |\bar{k}\rangle\langle\bar{k}| \qquad \text{e.g. } \varepsilon_{\bar{k}} = \frac{\hbar^2 \bar{k}^2}{2m}$$

$$\hat{V} = \sum_{\bar{q}\bar{k}} V_{\bar{k}\bar{q}} |\bar{k}\rangle\langle\bar{q}|$$

Green's functions



$$\boxed{\begin{aligned} \hat{G}(z) &= \frac{1}{z - \hat{H}} \\ \hat{G}_0(z) &= \frac{1}{z - \hat{H}_0} \end{aligned}}$$

$$z = \omega + i0^+$$

consider $G^{-1}(z) = z - \hat{H}$

$$\left[\hat{G}(z)^{-1}\right]_{\bar{k}\bar{q}} = \delta_{\bar{k}\bar{q}}\, z - \delta_{\bar{k}\bar{q}}\, \varepsilon_{\bar{k}} - V_{\bar{k}\bar{p}}$$

$$\hat{G}(z)^{-1} = \begin{pmatrix} z - \varepsilon_{k_1} & V_{k_2 k_1} & \cdots \\ V_{k_1 k_2} & z - \varepsilon_{k_2} & \\ \vdots & & \ddots \end{pmatrix}$$

In the diagona basis $\hat{H}|\alpha\rangle = \varepsilon_\alpha|\alpha\rangle$

$$G(z)_{\alpha\beta} = \frac{\delta_{\alpha\beta}}{z - \varepsilon_\alpha}$$

Compute

$$\boxed{\rho(\omega) := \lim_{\eta\to 0^+} -\frac{1}{\pi}\,\mathrm{Im}\,\underbrace{\mathrm{Tr}\left[\hat{G}(z=\omega+i\eta)\right]}} =$$

$$= -\frac{1}{\pi}\lim_{\eta\to 0^+} \mathrm{Im}\sum_\alpha \frac{1}{\omega-\varepsilon_\alpha+i\eta} =$$

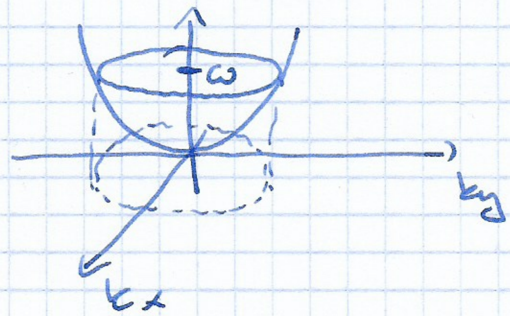
$$= \frac{1}{\pi}\lim_{\eta\to 0^+}\sum_\alpha \frac{\eta}{(\omega-\varepsilon_\alpha)^2+\eta^2} = \boxed{\sum_\alpha \delta(\omega-\varepsilon_\alpha)}$$

$\to \sum_\alpha \langle\alpha|\hat{G}(z)|\alpha\rangle = \sum_\alpha \frac{1}{z-\varepsilon_\alpha}$ - base independent

$$\boxed{\rho(\omega) = \sum_\alpha \delta(\omega-\varepsilon_\alpha)}$$

Density of states

How many $|\alpha\rangle$ states have energy (degenerate) $\varepsilon_\alpha = \omega$.



For continuum of states $\sum_k \to \int \frac{d_3 k}{(2\pi)^3}$

~~[illegible]~~

$\delta_{\bar{k}\bar{p}} \to \delta(\bar{k}-\bar{p})$

etc.

Formal solution for $\hat{G}(z)$

$$\hat{G}(z) = \frac{1}{z - \hat{H}_0 - \hat{V}} = \frac{1}{\hat{G}_0^{-1}(z) - \hat{V}} =$$

$$= \frac{1}{G_0^{-1}(z)} \frac{1}{1 - \hat{G}_0(z)\hat{V}} = \frac{\hat{G}_0(z)}{1 - \hat{G}_0(z)\hat{V}} =$$

$$= \hat{G}_0(z)\left[1 + \hat{V}\hat{G}_0(z) + \hat{V}\hat{G}_0(z)\hat{V}\hat{G}_0(z) + \cdots\right] =$$

$$= \hat{G}_0(z) + \hat{G}_0(z)\hat{V}\Big[\underbrace{1 + \hat{G}_0(z)\hat{V} + \hat{G}_0(z)\hat{V}\hat{G}_0(z)\hat{V} + \cdots}_{= \frac{1}{1 - \hat{G}_0(z)\hat{V}}}\Big]\hat{G}_0(z)$$

$$= \hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)$$

$$\boxed{\hat{T}(z) \equiv \frac{\hat{V}}{1 - \hat{G}_0(z)\hat{V}}}$$ T-matrix

$$\boxed{\hat{G}(z) = \hat{G}_0(z) + \hat{G}_0(z)\hat{T}(z)\hat{G}_0(z)}$$

a) Friedel sum rule

note $$\frac{\partial}{\partial z} \ln \hat{G}(z) = -\hat{G}(z)$$

proof $$\frac{\partial}{\partial z} \ln \frac{1}{z-\hat{\mathcal{H}}} = \ldots =$$

$$= -\frac{\partial}{\partial z} \ln (z - \mathcal{H}) = -\frac{1}{z-\mathcal{H}} = -G(z) \qquad \square$$

Also $$\rho(\omega) = \frac{1}{\pi} \frac{\partial}{\partial z} \operatorname{Im} \operatorname{Tr}[\ln G(z)]$$

We compute a change in DOS due to a scatterin center

$$\Delta\rho(\omega) = \rho(\omega) - \rho_0(\omega) =$$

$$= \frac{1}{\pi} \frac{\partial}{\partial z} \operatorname{Im} \operatorname{Tr}\left[\ln\left(\hat{G}(z) \cdot \hat{G}_0^{-1}(z)\right)\right] =$$

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

$$= \frac{1}{\pi} \frac{\partial}{\partial z} \operatorname{Im} \operatorname{Tr}\left[\ln\left(\hat{V}^{-1} \hat{T}(z)\right)\right]$$

Df. <u>Matrix of the scattering phase shifts</u>

$$\hat{\delta}(z) = \operatorname{Im} \ln\left(\hat{V}^{-1}\hat{T}(z)\right) = \operatorname{Arg}\left(\hat{V}^{-1}\hat{T}(z)\right)$$

hence, $$\boxed{\Delta\rho(\omega) = \lim_{\eta\to 0^+} \frac{1}{\pi} \frac{\partial}{\partial z} \operatorname{Tr}[\hat{\delta}(z)]}$$

Note, $|z| \to \infty$ $\quad G_0(z) \to \frac{1}{z} \to 0$, $\quad \hat{T}(z) \to \hat{V}$, $\quad \hat{\delta}(z) \to 0$

variation of the total number of states up to μ

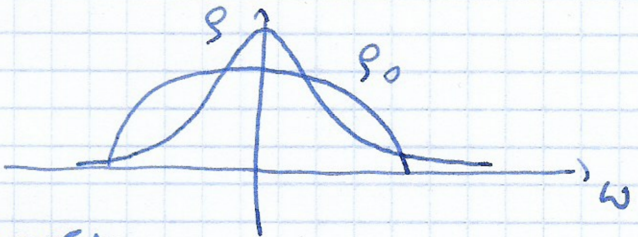
$$\boxed{\Delta N = \int_{-\infty}^{\mu} d\omega\, \Delta\rho(\omega) = \frac{1}{\pi} \mathrm{Tr}\, \hat{\delta}(\mu)}$$

Friedel sum rule

Note that for $\mu \to \infty$ $\quad \hat{\delta}(\pm\infty) = 0$

$$\Delta N = \int_{-\infty}^{\infty} d\omega\, \Delta\rho(\omega) = 0$$

Total number of states is not changed



areas are the same

o) optical theorem

From the definition of the $\hat{T}$-matrix

$$\hat{T}(z)^{-1} = [\hat{V}^{-1} - \hat{G}_0(z)]$$

$$[\hat{T}(z)^{-1}]^{+} = [\hat{V}^{-1} - \hat{G}_0(z^*)]$$

hence

$$[\hat{T}(z)^{-1}]^{+} - [T(z)^{-1}] = \hat{G}_0(z) - \hat{G}_0(z^*) \quad / \hat{T}^{+}(\ldots)\hat{T}$$

$$\hat{T}(z)^{+}\left[[T(z)^{-1}]^{+} - [T(z)^{-1}]\right]\hat{T}(z) = \hat{T}(z) - \hat{T}(z)^{+} =$$

$$= \hat{T}(z)^{+}\underbrace{[\hat{G}_0(z) - \hat{G}_0(z^*)]}_{-2\pi i \hat{\delta}(\omega - \hat{H}_0) \quad \eta \to 0^+}\hat{T}(z)$$

$\Rightarrow$

$$\boxed{T_{\bar k \bar q}(\omega) - T^{+}_{\bar k \bar q}(\omega) = -2\pi i \sum_{\bar p} T_{\bar k \bar p}(\omega)\, \delta(\omega - \varepsilon_{\bar p})\, T_{\bar p \bar q}(\omega)}$$

Optical theorem : Imaginary part of the T-matrix is finite only within the continuum band $\varepsilon_{\bar p} \in \mathbb{R}$.

•) S-matrix

Consider on-shell scattering with T-matrix

$$T_{\bar k \bar q}(\varepsilon) \quad \text{where} \quad \varepsilon = \varepsilon_{\bar k} = \varepsilon_{\bar q}$$

(elastic scattering which conserves the energy)

Rewrite optical theorem on-shell

$$-2\pi i\, \delta(\varepsilon_{\bar k} - \varepsilon_{\bar q}) \left[T^{+}_{\bar k \bar q}(\varepsilon) - T_{\bar k \bar q}(\varepsilon) \right] =$$

$$= (-2\pi i)^2\, \delta(\varepsilon_{\bar k} - \varepsilon_{\bar q}) \sum_{\bar p} T_{\bar k \bar p}(\varepsilon)\, \delta(\varepsilon_{\bar k} - \varepsilon_{\bar p})\, T_{\bar p \bar q}(\varepsilon)$$

Define S-matrix

$$\boxed{S_{\bar k \bar q}(\varepsilon) = \delta_{\bar k \bar q} - 2\pi i\, \delta(\varepsilon_{\bar k} - \varepsilon_{\bar q})\, T_{\bar k \bar q}(\varepsilon)}$$

Then it follows that S-matrix is unitary

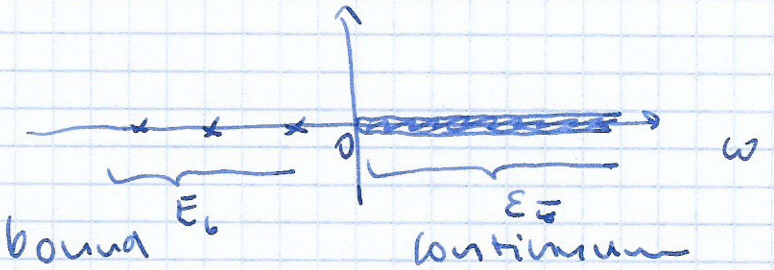
$$\boxed{\hat S \hat S^{+} = \mathbb{1}}$$

$S_{\bar k \bar q}(\varepsilon)$ – transition probability to scatter elastically from $|\bar k\rangle$ to $|\bar q\rangle$

•) Bound and continuum states

Levinson theorem

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



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

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 $\omega = E_b$

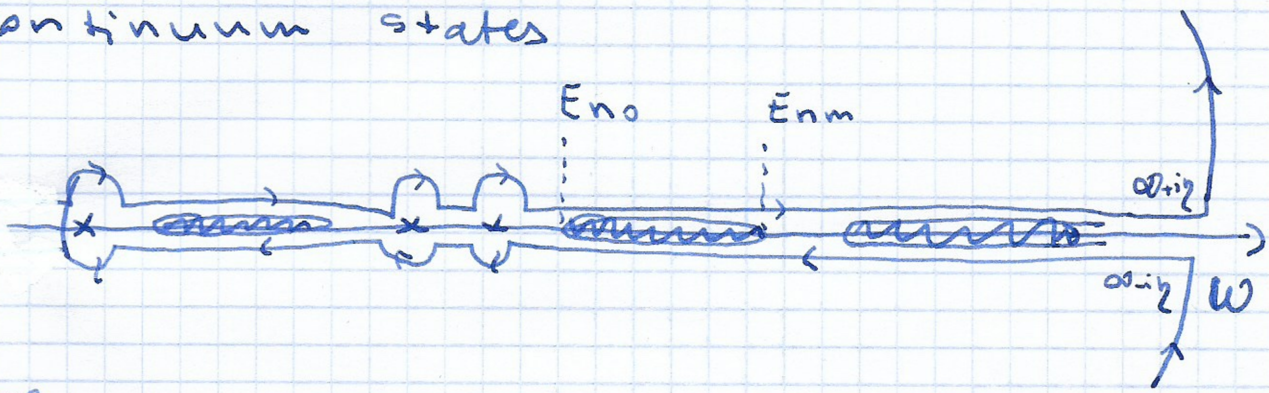
$$-\frac{1}{\pi}\, \mathrm{Im}\, \frac{d}{dz} \ln (z - E_b) \underset{\eta \to 0}{\rightarrow} \delta(\omega - E_b)$$

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

[number of bound states

$\square$

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



<u>Theorem</u>

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

if $f(z)$ analytic in and on C, appart 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 $\displaystyle \frac{1}{2\pi i} \oint_C \ln D(z)'\, dz = ?$

i) contributions from bound states

$$(i) = -N_b$$

ii) contributions along $\mathbb{R}$

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

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

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

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

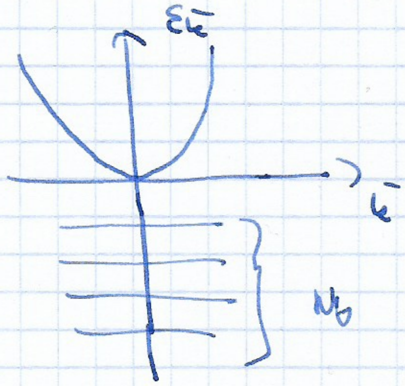
(iii) At ∞ $\quad \lim_{|\omega| \to \infty} D(\omega) = 1$ − finite on C_∞

Hence

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

Levinson theorem

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 →
→ resonance states discussion