Self-energy & decay rate: a tour in complex integration!

- Local Green-function and self-energy:

$$G_{xx}(z) = \langle x | \frac{1}{z-H} | x \rangle = \frac{1}{z - WV_x - \sigma_x(z)}$$

$z \in \mathbb{C}^+ = \{ z = E + i\eta,\ \eta > 0 \}$; x = site on a lattice of N sites

- $G_{xx}(z)$ singular when $\eta \to 0$ and E belongs to spectrum of H.
  It is analytic in $\mathbb{C}^+$.
  Can be represented as the integral of a measure $\nu_x(E)$, the "LOCAL DENSITY OF STATES":

$$G_{xx}(z) = \int_{E_{GS}}^{E_{max}} dE' \, \frac{\nu_x(E')}{z - E'}$$

For N finite, $\nu_x(E) = \sum_{\alpha=1}^{N} |\langle E_\alpha | x \rangle|^2 \, \delta(E - E_\alpha) > 0$

eigenvalues of H

eigenvectors of H.

- Local self-energies $\sigma_x(z)$ also analytic in $\mathbb{C}^+$.
  Can also be written as integral of a positive measure:

$$\boxed{\sigma_x(z) = \int_{E_{GS}}^{E_{max}} dE' \, \frac{\Gamma_x(E')}{z - E'}}$$

☒ At N finite, $G_{xx}(z)$ and $\sigma_x(z)$ have simple poles on real axis. When $N \to \infty$, poles coalesce into a branch cut.

☒ In class, we have seen that the return probability amplitude

$$A_x(t) = \Theta(t) \langle x | e^{-itH} | x \rangle = \lim_{\eta \downarrow 0} \frac{1}{2\pi i} \int_{\mathbb{R}} dE \, e^{-i(E+i\eta)t} G_{xx}(E+i\eta)$$

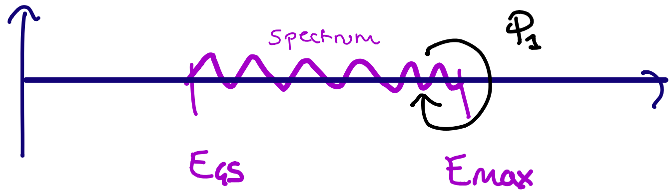
$$\stackrel{!}{=} \lim_{\eta \downarrow 0} \left(\frac{1}{2\pi i}\right) \int_{\mathbb{R}} dE \, e^{-iEt+\eta t} \frac{1}{E+i\eta - WV_x - \sigma_x(E+i\eta)}$$

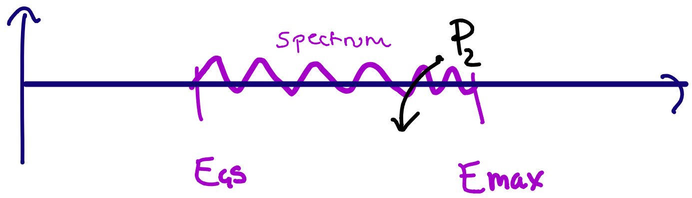
decays exponentially: $A_x(t) \sim A(t) e^{-\gamma t} + B(t)$ when $G_{xx}(z)$ has a pole z^* with a non-zero imaginary part, and the decay rate γ is related to imaginary part.

APPARENT PARADOX: $G_{xx}(z)$ has poles on the real axis (spectrum of H). How can it have poles that have imaginary part?

ANSWER: $G_{xx}(z)$, $\sigma_x(z)$ can have poles in "second Riemann sheet": see them when analytically-continue the function.

▨ When $N \to \infty$, $G_{xx}(z)$ develops a cut on real axis, in correspondence to the spectrum of H.





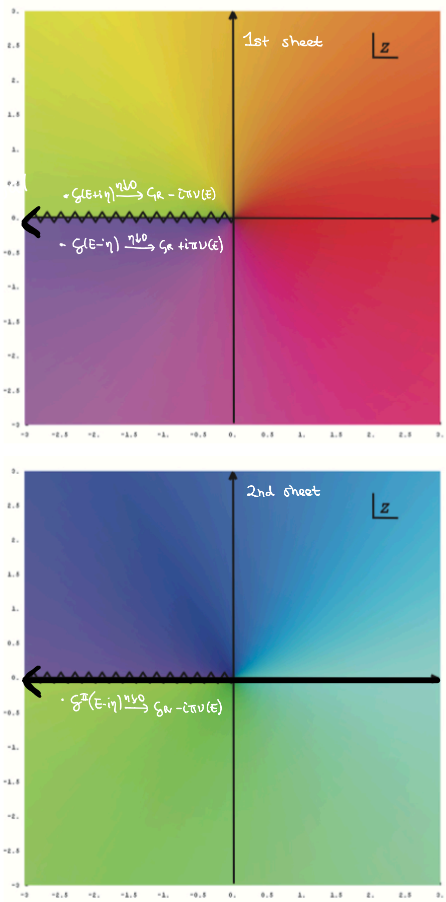
To analytically continue $G_{xx}(z)$ in region $z \in \mathbb{C}^-$, we can extend it along path P_1 that circles around branch point, or along P_2 that crosses the cut.

Because of cut, the function is multivalued (like $\sqrt{z}$) and the 2 analytic continuations are different:

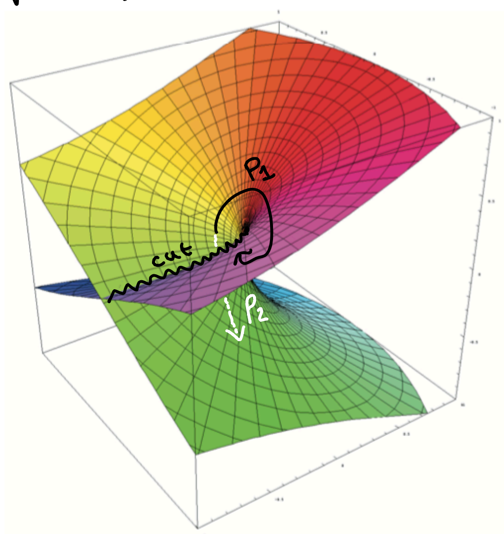
ANALYTIC CONTINUATION DEPENDS ON PATH!

The paths P_1 and P_2 bring us to two different regions of Riemann surface: P_2 to the "second Riemann sheet".
The analytic continuation along P_1 gives a discontinuity above and below the cut. The analytic continuation along P_2 is continuous across the cut.

Call $G_x^{I}(z)$, $\sigma_x^{I}(z)$ the analytic continuation along P_1, and $G_x^{II}(z)$, $\sigma_x^{II}(z)$ the one along P_2.



Riemann Surface

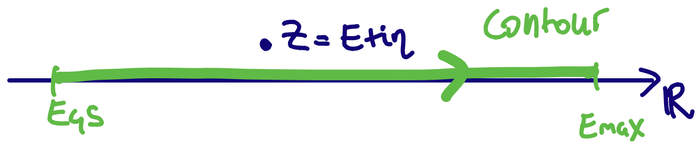


(Here spectrum is the negative real axis)

☒ $G^{II}_{xx}(z)$ is computed this way:

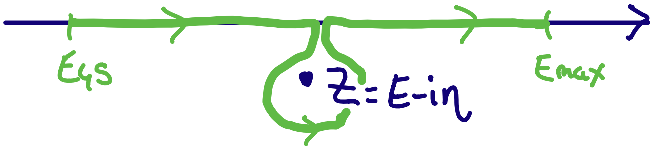
for $\operatorname{Im} z > 0$, $\displaystyle \mathcal{G}_{xx}(E+i\eta) = \int_{E_{GS}}^{E_{max}} dE' \, \frac{\nu_x(E')}{E+i\eta-E'}$ such that the

poles of integrand have positive imaginary part ($E'_{pole} = E + i\eta$)
and the integration contour is below them:



The contour can be deformed in $\mathbb{C}$, provided one does not cross singularities/poles.

To continue to $z \in \mathbb{C}^-$, need to modify the contour in such a way that remains below the pole:



The analytic continuation to $z \in \mathbb{C}_1^-$ is:

$$G^{II}_{xx}(z) = \underbrace{\int_{E_{GS}}^{E_{max}} dE' \, \frac{V_x(E')}{z-E'}}_{\text{contribution straight contour}} + \underbrace{2\pi i \lim_{E' \to z} (E'-z) \frac{V_x(E')}{z-E'}}_{\text{contribution of little circle}} = \int_{E_{GS}}^{E_{max}} dE' \, \frac{V_x(E')}{z-E'} - 2\pi i \, V_x(z)$$

The second contribution is not there in the analytic continuation along P_1: that contribution makes $G^{II}(z)$ continuous along cut.

The same holds for $\sigma_x(z)$: along P_2, the continuation gives:

$$\sigma^{II}_x(z) = \int dE' \, \frac{\Gamma_x(E')}{z-E'} - 2\pi i \, \Gamma_x(z) := \sigma_x(z) - 2\pi i \, \Gamma_x(z)$$

$$\Longrightarrow \quad g^{II}_x(z) = \frac{1}{z - WV_x - \sigma^{II}_x(z)} = \frac{1}{z - WV_x - \sigma_x(z) + 2\pi i \, \Gamma_x(z)}$$

can have poles with imaginary part!

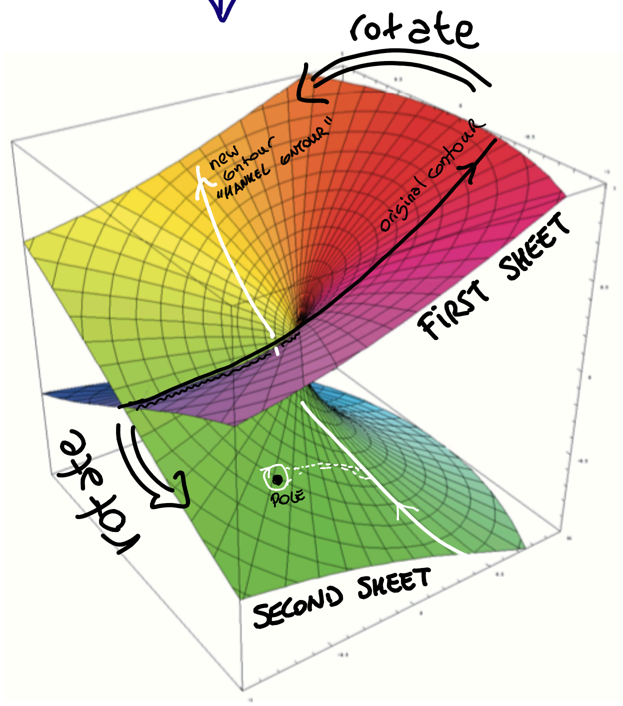
☒ The amplitude:

$$A_x(t) = \lim_{\eta \downarrow 0}\left(\frac{1}{2\pi i}\right)\int_{\mathbb{R}} dE\, e^{-iEt+\eta t}\,\frac{1}{E+i\eta - WV_x - \sigma_x(E+i\eta)}$$

$$= \lim_{\eta \downarrow 0}\frac{1}{2\pi i}\int_{\mathcal{B}} dz\,\frac{e^{-izt}}{z - WV_x - \sigma_x(z)}$$

$\mathcal{B} = \{z = E + i\eta,\ \eta > 0\}$

can be computed deforming the contour $\mathcal{B}$ as shown here: in this way, one gets the contribution of the pole in the 2nd sheet, that can be computed by Residue theorem and gives $A(t)\,e^{-\gamma t}$.



One also have a contribution from the white contour (Henkel contour) that gives a slower-decaying function $B(t)$.

Notice: perturbatively in the kinetic term t of the Anderson Hamiltonian, one finds

$$\gamma = \underbrace{\Gamma_x(WV_x)}_{\text{imaginary part of self-energy}} + \mathcal{O}(t^4) \implies \text{Fermi Golden rule!}$$