

Last week we discussed response functions

this week extend it to infinite systems and model absorption / dissipation and look at the time domain

discussed two examples:

- classical harmonic oscillator



- H atom



For ce on particle $\vec{F}_0 \cos \omega t$
on electron in electric field $e\vec{E}_0 \cos \omega t$
and potential $-\vec{F}_0 \cancel{\approx} \cos \omega t$

We have linear response as long as \propto small

$\Rightarrow F_0 \propto t$ small.

large forces that only act for a very short time still give linear response

(2)

For linear response we have

$$x = \chi(\omega) F$$

↓ ↓
 position susceptibility
 force

and $\chi(\omega) = \frac{\omega_0}{\omega^2 - \omega_0^2}$

with $\omega_0 = \sqrt{\frac{k}{m}}$ classical harmonic oscillator

$\omega_0 = E_p - E_s$ H-atom.

For a two level system we have:

$$\hat{x} = \begin{pmatrix} 0 & \mu_i \\ \mu_i & 0 \end{pmatrix} \quad \text{and } \mu_i = \langle \psi_i | \hat{x} | \psi_i \rangle$$

$$\hat{H}_0 = \begin{pmatrix} 0 & 0 \\ 0 & \omega_i \end{pmatrix}$$

$$H_1 = V \sin \omega t \hat{x}$$

$$H = H_0 + H_1$$

(3)

The solution linear in V is

$$\psi(t) = \psi_0 + \left[-ie^{-it\omega_i} \omega + iw \cos \omega t + \omega_i \sin \omega t \right] \psi_i$$

which one can proof by showing that

$$i\frac{d}{dt} \psi(t) = H(\psi(t)) \quad \text{upto linear order in } V$$

(neglect all terms with V^2)

The induced polarization is:

$$\begin{aligned} \sigma &= \langle \psi(t) | \hat{x} | \psi(t) \rangle \\ &= \frac{2V\mu_i^2}{(\omega^2 - \omega_i^2)} (\omega_i \sin \omega t - \omega \sin \omega_i t) \end{aligned}$$

and the susceptibility is

$$\begin{aligned} \chi &= \frac{2\mu_i^2}{\omega^2 - \omega_i^2} \\ &= \frac{\mu_i^2}{\omega - \omega_i} - \frac{\mu_i^2}{\omega + \omega_i} \end{aligned}$$

(4)

The susceptibility is purely real and the conduction $\sigma = -i\omega \chi$ purely complex with absorption $= \text{Re}[\sigma]$ we find there is no absorption. After some time a driven two level system returns to its starting position oscillations of energy but no absorption. let's see what happens if we go to an infinite system.

first look at a 3-level system

$$\hat{x} = \begin{pmatrix} 0 & \mu_1 & \mu_2 \\ \mu_1 & 0 & 0 \\ \mu_2 & 0 & 0 \end{pmatrix} \quad \begin{matrix} \mu_i: \text{dipole moment} \\ \text{between } \psi_0 \text{ and state } \psi_i \end{matrix}$$

$$H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \omega_1 & 0 \\ 0 & 0 & \omega_2 \end{pmatrix} \quad \begin{matrix} \omega_i: \text{eigen energy of} \\ \text{orbital } \psi_i \end{matrix}$$

$$H_1 = V \sin \omega t \hat{x}$$

$$H = H_0 + H_1$$

We solve $\psi(t)$ using a
guessed function for $\psi(t)$ that solves

$$i\frac{d}{dt}\psi(t) = H\psi(t) \quad \text{linear in } V$$

$$\psi(t) = \psi_0 + \frac{V\mu_1}{(\omega^2 - \omega_1^2)} \left(-ie^{-i\omega_1 t} (\omega + i\omega \cos \omega t + \omega_1 \sin \omega t) \right) \psi_1$$

$$+ \frac{V\mu_2}{(\omega^2 - \omega_2^2)} \left(ie^{-i\omega_2 t} (\omega + i\omega \cos \omega t + \omega_2 \sin \omega t) \right) \psi_2$$

and $x(t) = \langle \psi(t) | \hat{x} | \psi(t) \rangle$

$$= \frac{2V\mu_1}{(\omega^2 - \omega_1^2)} \sin \omega t + \frac{2V\mu_2}{(\omega^2 - \omega_2^2)} \sin \omega t$$

$$\chi(\omega) = \chi_1(\omega) + \chi_2(\omega)$$

$$= \frac{\mu_1^2}{\omega - \omega_1} + \frac{\mu_1^2}{\omega + \omega_1} + \frac{\mu_2^2}{\omega - \omega_2} - \frac{\mu_2^2}{\omega + \omega_2}$$

(6)

For a many level system we thus have

$$\chi_i(\omega) = \frac{\mu_i^2}{\omega - \omega_i} - \frac{\mu_i^2}{\omega + \omega_i}$$

$$\text{and } \chi(\omega) = \sum_i \chi_i(\omega)$$

$$\text{as } \hat{x}|q_0\rangle = \sum_i \mu_i |q_i\rangle$$

$$\text{and } \frac{1}{\omega - \omega_0} |q_0\rangle = \frac{1}{\omega - \omega_i} |q_i\rangle$$

we have

$$\langle q_0 | \hat{x} \frac{1}{\omega - \omega_0} \hat{x} | q_0 \rangle = \sum_{ij} \langle q_j | \mu_j \frac{1}{\omega - \omega_i} \mu_i | q_i \rangle$$

$$= \sum_i \frac{\mu_i^2}{\omega - \omega_i}$$

or

$$\chi(\omega) = \langle q_0 | x \frac{1}{\omega - \omega_0} x | q_0 \rangle - \langle q_0 | x \frac{1}{\omega + \omega_0} x | q_0 \rangle$$

(7)

We derived it for H and x on eigen basis
but formula is basis independent, i.e. true
for any set of states

with $u^* u = 1$ we have

$$\langle \psi_0 | x u^* u^T \xrightarrow{w-H} u^* u^T x | \psi_0 \rangle$$

$$= \langle \psi_0 | x u^* \xrightarrow{\frac{1}{u^*(w-H)u^T}} u^T x | \psi_0 \rangle$$

$$= \langle \psi_0 | u^* u^T x u^* \xrightarrow{\frac{1}{w - u^* H u^T}} u^T x u^* u^T | \psi_0 \rangle$$

$$= \langle \psi_0 | u^T \psi_0 | u^T x u^* \xrightarrow{\frac{1}{w - u^* H u^T}} u^T x u^* | u^T \psi_0 \rangle$$

i.e. form valid for any basis set.

(8)

But we still have the problem that

$$\chi(\omega) = \sum_{i=1}^N \frac{\omega_i^2}{\omega - \omega_i} - \frac{\omega_i^2}{\omega + \omega_i}$$

is purely real i.e. or purely complex
and dissipation or $\text{Re}[\sigma]$ i.e. $= 0$

Now let's take the limit of N to ∞ ...

in such a way that total coupling not diverges.

N levels from ω_{\min} to ω_{\max}

$$\text{Spacing } \Delta\omega_0 = \frac{\omega_{\max} - \omega_{\min}}{N}$$

$$\omega_i = \omega_{\min} + (i + \frac{1}{2}) \Delta\omega_0$$

$$i \in [0, N]$$

(9)

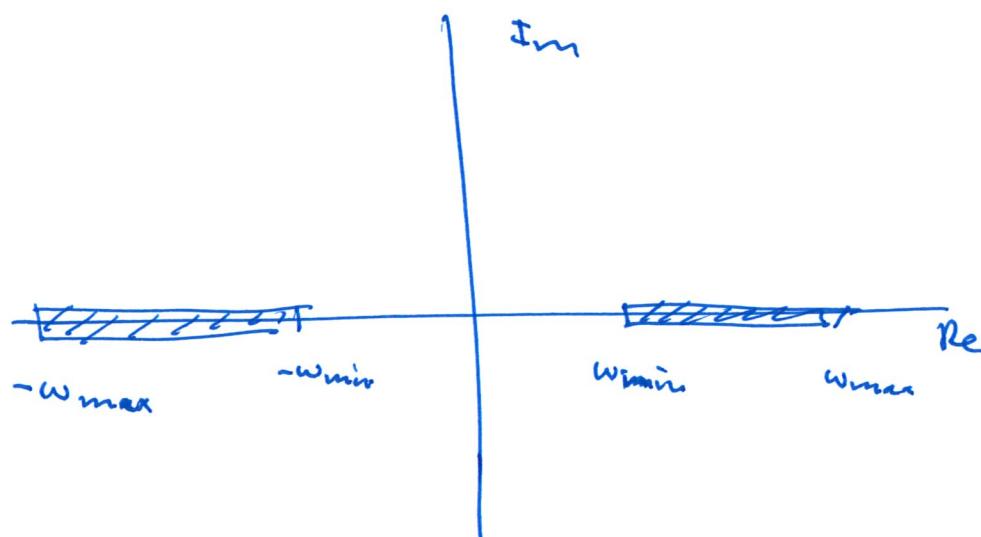
Coupling strength : $\mu_i = \mu \sqrt{\omega_0}$

$$\chi = \sum_{i=1}^N \mu^2 \omega_0 \left(\frac{1}{\omega - \omega_p} - \frac{1}{\omega + \omega_i} \right)$$

for $N \rightarrow \infty$ this becomes

$$\chi(\omega) = \int_{\omega_{\min}}^{\omega_{\max}} \mu^2 \left(\frac{1}{\omega - \omega_0} - \frac{1}{\omega + \omega_0} \right) d\omega_0$$

pole when $\omega_{\min} < |\omega| < \omega_{\max}$

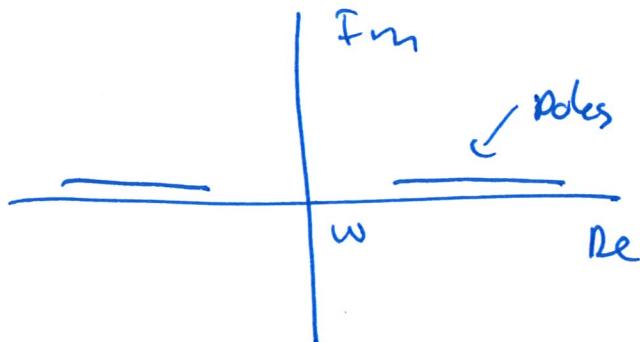


(10)

Shift poles by small energy η in the imaginary plane and take $\eta \rightarrow 0$

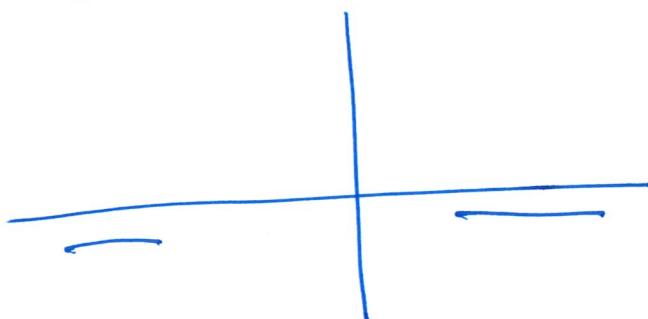
4- options

η negative



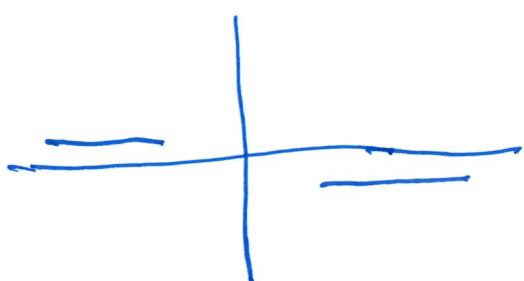
Advanced Green's / Response Functions

η positive



Retarded

change sign of η depending if $w > 0$ or $w < 0$



Causal or Feynman.

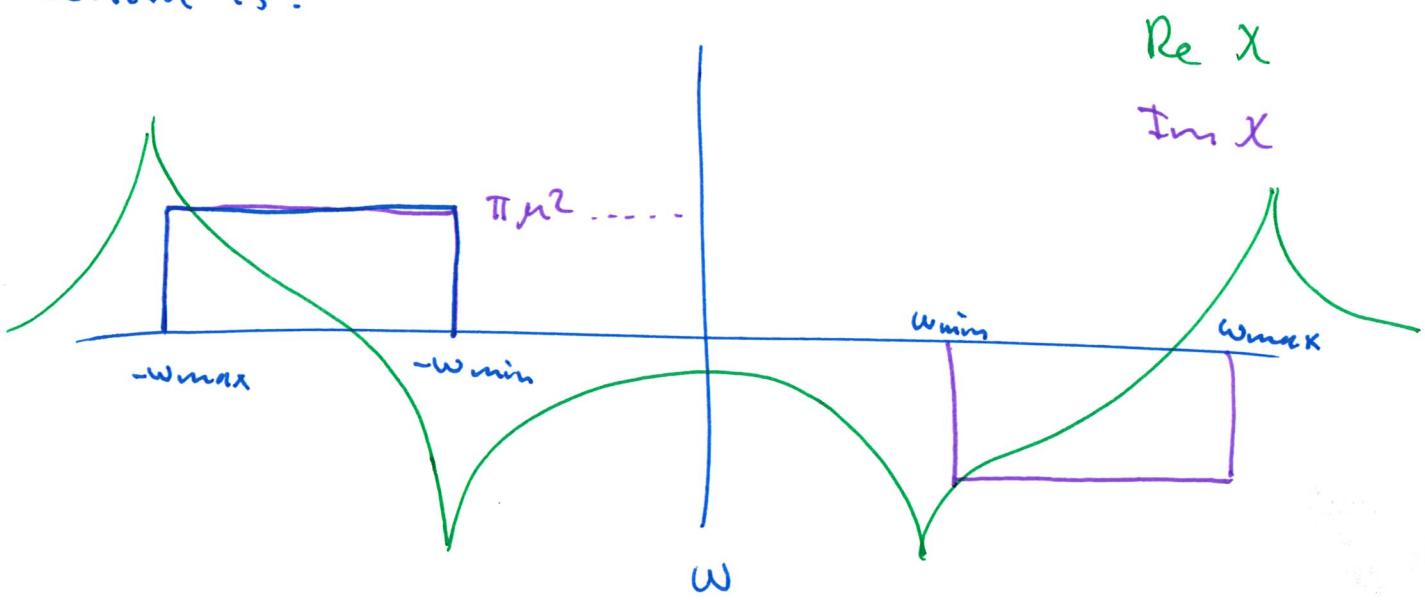
(11)

The Retarded phase definition is consistent with our classical result (γ for damping)

and we have

$$\chi(\omega) = \lim_{\eta \rightarrow 0^+} \left[\int_{\omega_{\min}}^{\omega_{\max}} \mu^2 \left(\frac{1}{\omega - \omega_0 + i\eta} - \frac{1}{\omega + \omega_0 + i\eta} \right) d\omega_0 \right]$$

which is:



The result is a complex function $\Rightarrow \text{Im}(\chi(\omega))$

No tangy zero \Rightarrow dissipation

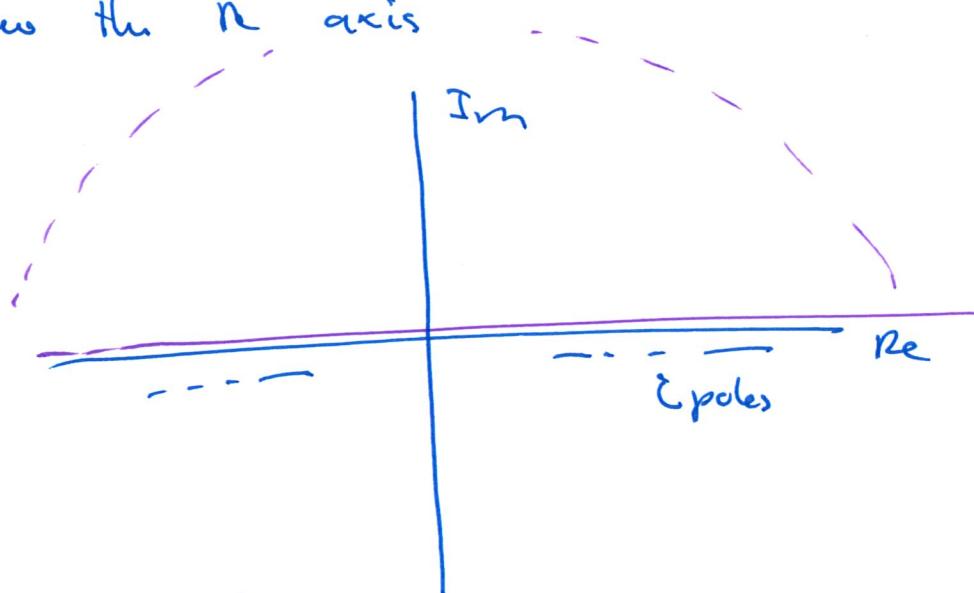
Kramers-Kronig relations

$\text{Re}[\chi]$ and $\text{Im}[\chi]$ are related.

If you know one you know the other

In the complex plane $\chi(w)$ has poles

below the Re axis



an integral over the upper half plane

$\oint \chi(w) dw = 0$ thus yields zero

$\chi(\text{Im} w \rightarrow \infty) = 0$ such that the integral over
the arc = 0 and

$$\int_{-\infty}^{\infty} \chi(w) dw = 0$$

(13)

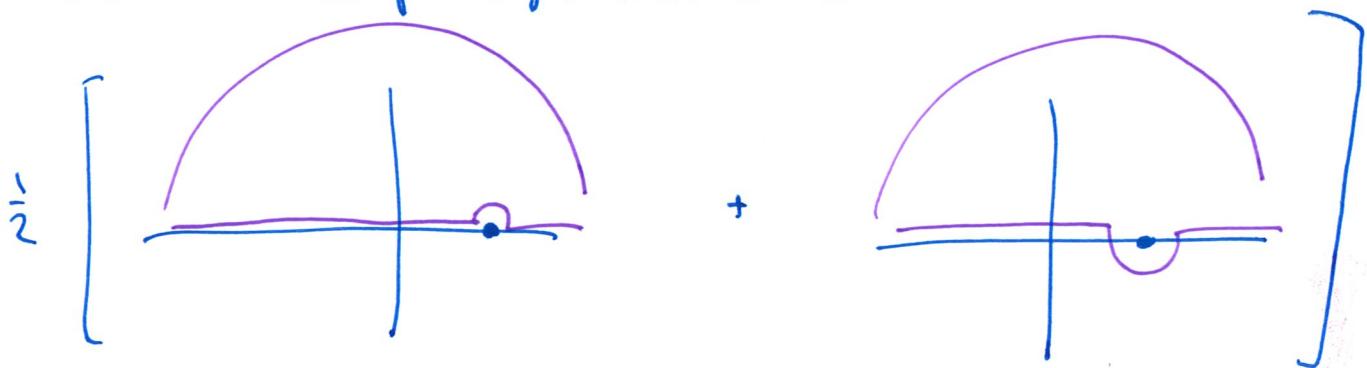
and $\chi(\omega)$ for $\operatorname{Im}(\omega) > 0$ is analytical

If we now look at

$\operatorname{Pf} \int \frac{\chi(\omega)}{\omega - \omega_0} d\omega$ then the contour

crosses a pole at $\omega = \omega_0$

we take the principal value as



$$\text{or } \operatorname{Pf}_{-\infty}^{\infty} \frac{\chi(\omega)}{\omega - \omega_0} d\omega = \pi i \operatorname{Res}_{\omega_0} \frac{\chi(\omega)}{\omega - \omega_0} = \pi i \chi(\omega_0)$$

we thus have

$$\operatorname{Pf}_{-\infty}^{\infty} \frac{\chi(\omega)}{\omega - \omega_0} d\omega = \pi i \chi(\omega_0) \text{ or}$$

$$\operatorname{Pf}_{-\infty}^{\infty} \frac{\operatorname{Re}[\chi(\omega)]}{\omega - \omega_0} d\omega = -\pi \operatorname{Im} \chi(\omega_0)$$

(14)

$$P \int_{-\infty}^{\infty} \frac{Im[\chi(\omega)]}{\omega - \omega_0} d\omega = +\pi Re \chi(\omega_0)$$

Response function in the time domain.

(15)

$$X(\omega) = \left(\frac{1}{\omega - \omega_0 + i\eta} T(\psi_0) - \frac{1}{\omega + \omega_0 - i\eta} T(\psi_0) \right)$$

gives the response of a system for an oscillating

force $F = F_0 \sin \omega t$

in general $F(t)$ could be any function

we can always write

$$F(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) e^{-i\omega t} d\omega$$

$$\text{or } F(\omega) = \int_{-\infty}^{\infty} f(t) e^{i\omega t} dt$$

amplitude of the force at frequency ω

for each frequency we have

$$x(\omega) = X(\omega) F(\omega)$$

with

$$F = F(\omega) e^{-i\omega t}$$

$$x = x(\omega) e^{-i\omega t}$$

for oscillations at a single frequency.

In order to calculate $x(t)$ for a general force $F(t)$ we can use that

$$\text{if } h(x) = \int_{-\infty}^{\infty} f(y) g(x-y) dy$$

then

$$\int_{-\infty}^{\infty} h(x) e^{-ixt} dx = \int_{-\infty}^{\infty} f(x) e^{-ixt} dx \int_{-\infty}^{\infty} g(x) e^{-ixt} dx$$

i.e. The Fourier transform of a convolution is the product of two Fourier transforms

(17)

$$\text{For } x(t) = \int_{-\infty}^{\infty} \chi(\tau) F(t-\tau) d\tau$$

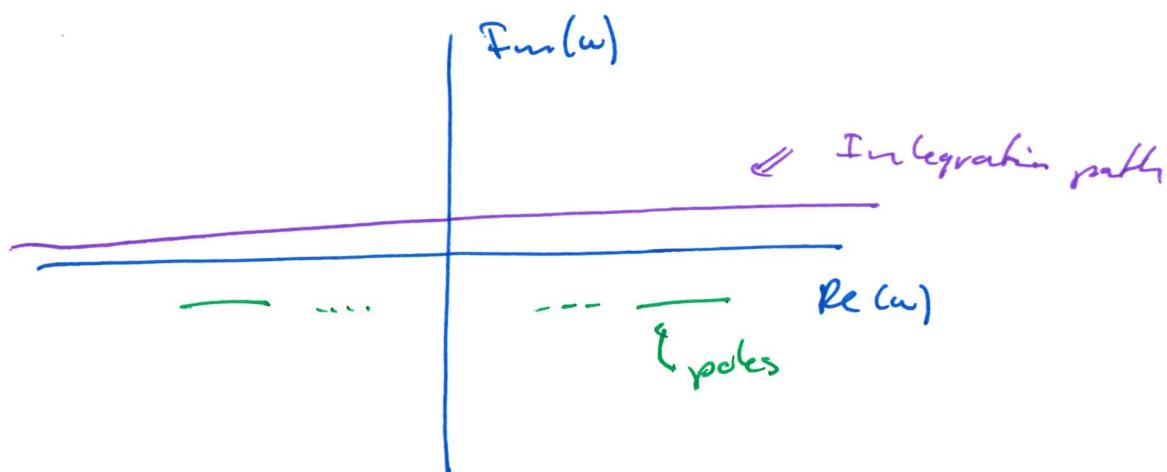
we have

$$\begin{aligned} x(\omega) &= \int_{-\infty}^{\infty} x(t) e^{i\omega t} dt \\ &= \int_{-\infty}^{\infty} \chi(\tau) e^{i\omega t} dt \int_{-\infty}^{\infty} F(t) e^{i\omega t} dt \\ &= \chi(\omega) F(\omega) \end{aligned}$$

$$\text{with } \chi(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} x(t) e^{-i\omega t} dt$$

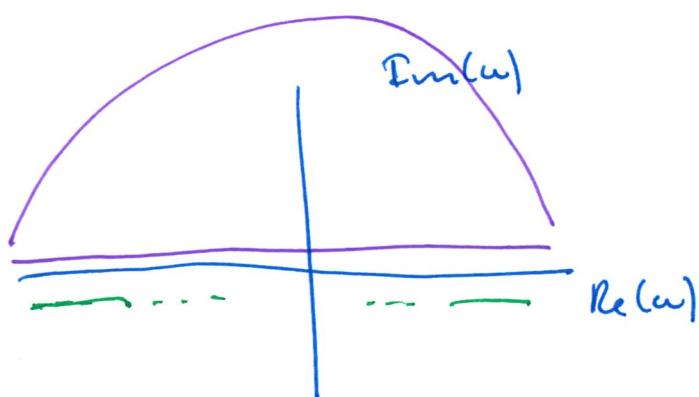
$\chi(\omega)$ has poles in the negative / lower complex half plane. We can use residue calculus to solve the integral.

We have poles at $\omega = \hbar - E_0 + i\omega t$
and $\omega = -\hbar + E_0 + i\omega t$



We can close the integration path either in the upper or lower half plane

Closing in the upper half yields



$$\int_{\text{upper half}} e^{-i\omega t} \left(\langle \psi_0 | \frac{1}{\omega + H - E_0 + i\omega t} | \psi_0 \rangle - \langle \psi_0 | \frac{1}{\omega + H - E_0 + i\omega t} | \psi_0 \rangle \Big|_{\omega=0} \right) d\omega = 0$$

(19)

while no poles are enclosed in the contour
we thus have

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iwt} X(\omega) d\omega = -\frac{1}{2\pi} \int_{\text{arc}} e^{-iwt} X(\omega) d\omega$$

on the arc $\text{Im}(\omega) > 0$ the exponent thus
behaves as $e^{i\text{Im}(\omega)t}$

for $t < 0$ and $|\omega| \rightarrow \infty$ this goes to zero

thus $X(t < 0) = 0$

By similar arguments the integral over the lower
arc is zero for positive times. The integral over
the contour in the lower half complex plane
is equal to the residues such that we have

$$X(t) =$$

$$\frac{1}{2\pi} \int_{\text{lower half}} X(\omega) e^{-iwt} d\omega =$$

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-iwt} X(\omega) d\omega =$$

20

Residue of $\frac{1}{2\pi} e^{-i\omega t} \langle \psi_0 | T \frac{1}{\omega - H + i\eta} T | \psi_0 \rangle$

$$-\frac{1}{2\pi} e^{-i\omega t} \langle \psi_0 | T \frac{1}{\omega + H - E_0 + i\eta} T | \psi_0 \rangle$$

$$x(t) = e(t) i \left[\langle \psi_0 | T e^{-i(H-E_0)t} T | \psi_0 \rangle - \langle \psi_0 | T e^{i(H-E_0)t} T | \psi_0 \rangle \right]$$

$$= \Theta(t) i \left[\langle \psi_0 | e^{iE_0 t} T e^{-iHt} T | \psi_0 \rangle - \langle \psi_0 | T e^{iHt} T e^{-iE_0 t} | \psi_0 \rangle \right]$$

$$= \Theta(t) i \left[\langle \psi_0 | T(t) T(t=0) | \psi_0 \rangle - \langle \psi_0 | T(t=0) T(t) | \psi_0 \rangle \right]$$

In order to get a better understanding of $\chi(t)$ we can have a look at the response to a delta function (short peak, clap or explosion)

$$F(t) = \delta(t)$$



the response will be:

$$x(t) = \int_{-\infty}^{\infty} \chi(\epsilon) F(t-\epsilon) d\epsilon$$

$$= \chi(t)$$

for a two level system or classical Harmonic Oscillator this is

$$e(t) i [e^{-i\omega_0 t} - e^{i\omega_0 t}] e^{-\eta t}$$

with $\omega_0 = \omega_i - \omega_0$ the energy difference between excited and ground state

$$x(t) = \Theta(t) * e^{-\eta t} \sin(\omega_0 t)$$

