

# **Mathematics of Causality- Simplified Deliberation**

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## **Abstract**

Strike a bell, and then hear sound not before striking. This is statement of causality is Universal phenomena. The information about theory of Causality is too scattered, and is not concise, and is lost in complex analysis-making the understanding complicated. In the literature authors use mathematical formulas without explaining them thoroughly, and their practical utility. The purpose of this lecture note is to make stringent presentation of the principles of causality-develop the mathematics in a simplified way, and still make the purpose of applications in mind. A simple principle of nature that effect can only happen after cause, i.e. called causality has great mathematical treatment and development we term that as Kramer-Kronigs relation, analyticity, Titchmarsh principle etc. Like the statement- ‘a causal response function is analytic in upper-half of the complex plane’-sounds very complicated and philosophical. Though in complex-analysis terms these causality principles looks very complicated here in this note we simplify the derivation of analyticity Kramers-Kronigs relations and obtain these expressions in time and frequency domains. We start from the basics of Impulse Response Function or Green’s Function and then define the generalized susceptibility. From there we elaborate by use of Fourier transformation techniques the Kramer-Kronig relations in frequency domain and also in time domain. This method gets applied to various fields, i.e. in impedance studies, in dielectric relaxation/retardation studies, in refractive index studies, in electric polarization studies, in magnetic systems studies, in stress-strain relaxation studies etc. Even we if we make an artificial material with negative permittivity and negative permeability (thus showing negative refraction), it should and must follow the mathematical tests of causality that is Kramer-Kronigs relation. This note the examples we consider are for Debye systems, however, the theory and principles can be extended to non-Debye systems. We are not sure about causality theory that is developed and discussed here if it can be applied to non-differentiable systems i.e. response function defined on fractal support? –perhaps a new formal mathematics needs to be developed in this regard. Our discussion is only for continuous and differentiable systems.

## **Keywords:**

Susceptibility, Impulse Response Function, Hilbert-transform, Fourier Transform, Conjugate Fourier Transform, Convolution, Causal systems, non-Causal systems, Analyticity, Kramer-Kronigs relation

## 1. Introduction

Many observable quantities obey the Kramer-Kronig relations. For instance the electric susceptibility describes the electric polarization of a material responds to an applied electric field. This response must be causal so the real and imaginary parts of the electric susceptibility must be related by the Kramer-Kronig relations. This is also true for the magnetic susceptibility, the electrical conductivity, the thermal conductivity, and the dielectric constant, strain and stress compliance functions. Even we if we make an artificial material with negative permittivity and negative permeability (thus showing negative refraction), it should and must follow the mathematical tests of causality that is Kramer-Kronigs relation. We discuss the very simple statement that causality in time domain for a response function means analyticity in the upper half of complex frequency domain. Sometimes it is experimentally easier to measure the real part (or the imaginary part) of the susceptibility. The Kramer-Kronig relations can then be used to calculate the part that is difficult to measure. If both real and imaginary parts can be measured, it is possible to check for experimental errors using the Kramer-Kronig relations. If susceptibility is calculated theoretically, it is a good idea to check and see if it satisfies the Kramer-Kronig relations. It is considered a serious error to present a result that violates causality. The Kramer-Kronig relations describe how the real and imaginary parts of the susceptibility are related to each other. If either the real part or the imaginary part of the susceptibility is known for positive frequencies the entire susceptibility can be calculated at all frequencies (negative as well as positive). In this note we start with basics of Greens function, i.e. impulse response function, and then develop the concept of susceptibility in time domain. We then take the idea of susceptibility and compose the causal Green's function in time domain, by non-causal even and odd functions, and then derive the relation of these parts. We see that the non-causal components are the Hilbert Transform of each other in time domain, and doing the Fourier transformation of these relations we arrive at Kramer-Kronigs relation in frequency domain. This frequency domain representation of Kramer-Kronigs relation are usual integral representations relating real part of susceptibility to the imaginary part of susceptibility function. We take example of mechanical system, a single time constant system a Debye type and derive the shear compliance and then dynamic shera compliance by Forier Transformation of the Green's function-and then we draw equivalence to Electrical system, for dielectric relaxation (or retardation). This note will be helpful as it deals with detailed derivations and explanations that are lost in literature of Kramer-Kronigs relations and complex analysis.

## 2. Impulse Response of System

Consider a linear device (a linear system), which is supplied with an input field a function i.e. time varying call it  $f(t)$  and as a result the device gives output  $x(t)$ . Assume the input field  $f(t')$  is applied at a time  $t'$  is sustained for a short infinitesimal period call it  $dt'$  and we say output of the system at some later time  $t > t'$  is proportional to input field, i.e. in the form

$$dx(t) = (\chi(t, t'))(f(t')dt')$$

with proportionality term as function  $\chi(t, t')$ . Hence, the function  $\chi(t, t')$  describes the operation of a linear device or linear system.

The application of input field can be anywhere in time axis  $t' \in (-\infty, \infty)$ . Similarly the measured response can be anywhere in time axis  $t \in (-\infty, \infty)$ , but with condition that is  $t > t'$ . Assuming this operation has no explicit dependence (i.e. no in-built clock that changes its behavior) then the relation between the input and the output will only depend on the time interval i.e.  $t - t'$  and not on the absolute time i.e.  $t$ . Therefore, we may replace the function  $\chi(t, t')$  with a function of single variable i.e.  $\chi(t - t')$ ; i.e. we

have  $\chi(t-t') \leftarrow \chi(t, t')$ . This  $\chi(t-t')$  is called response function of system, or fundamental impulse response; or linear response coefficient; or susceptibility. The general method of describing  $\chi(t)$  is description in frequency domain, and the complex function that describes susceptibility is  $\chi(\omega)$ . Why  $\chi(t-t')$  is termed as impulse response is because we will see, that response of the system (or output) is  $x(t) = \chi(t)$  when the forcing function  $f(t) = \delta(t)$  i.e.  $\chi(t)$  is the response of system when excitation is unit delta function. This impulse response  $\chi(t)$  is also called Green's function.

We note here that determination of Green's function  $\chi(t)$  of system dynamic is very important, as we will see the Fourier transforming that Green's function, gives complex function called dynamic-susceptibility,  $\chi(\omega)$  and its complex conjugate  $\bar{\chi}(\omega)$ . Experimentally giving excitation as  $f(t) = \delta(t)$  is however, many a times difficult (except you strike a bell once that is delta function or you give a small duration pinch to body is delta function). In those cases we give step input excitation,  $f(t) \sim u(t)$  and get output  $y(t)$ , then by differentiation of this output response, we get the Green's function  $\chi(t)$ .

The concepts presented above are empirical descriptions of phenomena, that are the concept of a primary response function or susceptibility  $\chi(t)$ . It is like a time dependent shear compliance  $J(t)$ , time dependent permittivity  $\varepsilon(t)$ , time dependent magnetic permeability  $\mu(t)$  time dependent shear modulus  $G(t)$ , time dependent Electric Modulus  $M(t)$  or a time dependent magnetic susceptibility  $\chi_m(t)$  or time dependent electric-susceptibility  $\chi_e(t)$  etc. that do not involve understanding a given material, but are just general functions within which a discussion of the response to perturbation can be considered in a generic sense. All the above measured time dependent response functions  $J(t)$ ,  $\varepsilon(t)$ ,  $\mu(t)$ ,  $G(t)$ ,  $M(t)$ ,  $\chi_m(t)$ ,  $\chi_e(t)$  are experimentally obtained in relaxation (or retardation) experiments, by step-input excitation. In order to obtain the Green's function, one has to differentiate the same, and proceed to get dynamic quantities in the frequency domain. That we will elaborate in various cases. The experiments also give where ever possible, the frequency dispersion of the above quantities, that we will discuss subsequently.

### 3. Causality

Strike a bell and then hear its sound and not the other way round, is simply the principle of Causality. This is daily observed natural phenomena. The assumption of 'causality', namely that effect is after the cause, implies that output  $x(t)$  at any time  $t$  is obtained only due to input at or before  $t$ . Hence the expression  $dx(t) = (\chi(t-t'))(f(t')dt')$  applies only for  $t \geq t'$ , or equivalently  $\chi(t, t') = 0$  for  $t' > t$  or we say  $\chi(t-t') = 0$  for  $t' > t$ . We get the total output at any time  $t \in (-\infty, \infty)$  by integration of  $dx(t) = (\chi(t, t'))(f(t')dt')$  from application of input field at time  $t' = -\infty$  to  $t' = \infty$  (since,  $\chi(t, t') = 0$  when  $t' > t$ : i.e. 'the cause cannot be preceding the effect'). We express as follows the causality principle

$$x(t) = \int_{-\infty}^{\infty} \chi(t-t')f(t')dt'$$

The above is convolution operation of output function and input function  $x(t) = \chi(t) * f(t)$ . Where in convolution operation is denoted as (\*) and the convolution of two functions  $f_1(t)$  and  $f_2(t)$  is described

as  $f_1(t) * f_2(t)$  is  $\int_{-\infty}^{\infty} (f_1(t-t'))(f_2(t'))dt'$  or  $\int_{-\infty}^{\infty} (f_1(t'))(f_2(t-t'))dt'$ . We note that in frequency-transformed (Laplace Transformed) domain we have  $\mathcal{L}\{f_1(t) * f_2(t)\} = \mathcal{L}\{f_1(t)\} \mathcal{L}\{f_2(t)\}$ .

If the application of input is at time  $t' = 0$  then in  $x(t) = \int_{-\infty}^{\infty} \chi(t-t')f(t')dt'$  we have output at time after  $t > t'$  described as

$$x(t) = \int_0^t \chi(t-t')f(t')dt'$$

Note here the upper-limit is  $t' = t$ . If we change the variable calling it  $t-t' = \tau$ , then we have following

$$\begin{aligned} x(t) &= \int_0^t \chi(t-t')f(t')dt' = \int_t^0 \chi(\tau)f(t-\tau)(-d\tau) \\ &= \int_0^t \chi(\tau)f(t-\tau)d\tau \end{aligned}$$

While in equilibrium, the system is invariant in time-that we call steady state condition. Therefore the response at time  $t$  can only depend on the interval  $t-t'$  between the time of measurement  $t$  and the time  $t'$  at which the input field acts. Before the input field  $f(t')$  is applied there can be no response (this is “principle of causality”). Suppose that input field is unit impulse, i.e.  $f(t) = \delta(t)$  then

$$x(t) = \chi(t)$$

This implies  $\chi(t)$  is the response at time  $t$  to a unit impulse applied at time  $t = 0$ . This we have described in the previous section and this  $\chi(t)$  is called Green’s function too. By principle of causality,  $\chi(t) = 0$  for negative times i.e. for  $t < 0$ . The forcing delta function, is like strike bell once, and then you hear the ring, is impulse response, and its ringing is Green’s function. For a case of  $f(t) = u(t)$  the unit-step-input, say we have the response  $y(t)$  as following

$$\begin{aligned} y(t) &= \int_{-\infty}^{\infty} \chi(t-t')u(t')dt' = \chi(t) * u(t) \\ \frac{dy(t)}{dt} &= \frac{d}{dt}(\chi(t) * u(t)) \\ &= \chi(t) * \left(\frac{du(t)}{dt}\right) = \chi(t) * \delta(t) \\ \chi(t) &= \frac{dy(t)}{dt} \end{aligned}$$

We have used derivative of convolution as  $(f_1 * f_2)^{(1)} = f_1^{(1)} * f_2 = f_1 * f_2^{(1)}$ , in above steps. Therefore if we excite a system with an unit step function, then the derivative of response of that step input gives the Green’s function.

#### 4. Revising Green’s Function of a system

Consider a particle of mass  $m$  moving in a viscous fluid. The linear first order differential equation that describes this system is following

$$m \frac{dv(t)}{dt} + bv(t) = f(t)$$

Here  $b$  is the damping constant,  $v$  is the velocity, and  $f(t)$  is a driving force. A special case for the driving force is a  $\delta$ -function force which strikes the system at  $t = 0$ . Only after the force is struck, the system starts responding at  $t \geq 0$ , given by function  $v(t)$ . We assume  $v(t) = 0$  for  $t < 0$ . The solution to the differential equation for a  $\delta$ -function drive force is called the ‘impulse response function’-we called as  $\chi(t)$ . This is also called Green’s function. So we write the above dynamic equation as follows, in terms of greens function  $v(t) \leftarrow \chi(t)$  i.e. response to delta function as input  $f(t) \leftarrow \delta(t)$ .

$$m \frac{d\chi(t)}{dt} + b\chi(t) = \delta(t)$$

The solution to this equation (or the Green’s function) is following

$$\chi(t) = \frac{1}{m} e^{-t/\tau}; \quad \tau = \frac{m}{b}; \quad t \geq 0$$

Where  $\tau$  is called the decay time-is also called ‘Time-Constant’. The velocity equation i.e. equation of motion as given above has counter parts in Electric field relaxation phenomena described as

$$\tau\epsilon \frac{d\mathbf{E}(t)}{dt} + \epsilon\mathbf{E}(t) = \mathbf{D}(t)$$

Where  $\mathbf{E}$  is Electric Field, which is Potential per unit distance  $\mathbf{E} = V / d$ ,  $\mathbf{D}$  is Dielectric Displacement of charges described as  $\mathbf{D} = Q / A$ . Where  $Q$  is the charge, and  $A$  is electrode area, the  $V$  is the potential across the electrode plates separated by dielectric of distance  $d$ . We have for a dielectric system  $\mathbf{D} \equiv (Q / A) \propto (V / d) \equiv \mathbf{E}$ ; or  $\mathbf{D} = \epsilon\mathbf{E}$ . This Electric Field Relaxation Equation also has a relaxing electric-field  $\mathbf{E}(t) = \frac{1}{\epsilon\tau} e^{-t/\tau}$ , for  $t \geq 0$  with unit-impulse forced Dielectric Displacement,  $\mathbf{D}(t) = \delta(t)$  as applied as forcing function at  $t = 0$ ; with condition  $\mathbf{E}(t) = 0$  for  $t < 0$ . Thus Green’s function in this case is  $\chi(t) = \frac{1}{\epsilon\tau} e^{-t/\tau}$ .

Thus system Green’s function gives the characteristic response or impulse response function. This  $\chi(t)$  the Green’s function is always ‘decaying type of function’-may be exponentially decaying, stretched exponential decaying function, may be decaying like power law, may be decaying as damped oscillatory function, or even may have sustained oscillation, may be decaying as per Mittag-Leffler function. The equation of motion and Electric field relaxation that we considered a first order differential equation describes single-time constant simple relaxation systems, and are called “Debye relaxation”. There could be complex relaxation phenomena too.

This Green’s function  $\chi(t)$  or impulse response function will however never be growing type, and will be effective only at  $t \geq 0$  and will be zero for  $t < 0$ . This is causality, i.e. cause will always preceded the

effect. The cause is forcing function and effect is ‘relaxation’ of  $v(t)$  or  $\mathbf{E}(t)$ , in our two described system-by first ordered differential equations. We can also have second order, or fractional order systems, and those will have different Green’s function; however for causal system it will be always decaying type. Generally thus we have in general  $\lim_{t \rightarrow \infty} \chi(t) = 0$ , where  $\chi(t)$  is Green’s function of system.

## 5. Use of Green’s Function

The utility of the ‘impulse response function’ is that any driving force can be thought of as being built up of many  $\delta$  function forces.

$$f(t) = \int_{-\infty}^{\infty} \delta(t-t')f(t')dt'$$

The above integral is property of delta function. In convolution expression, the above integral is expressed as  $f(x) = \delta(x) * f(x)$  i.e.

$$f(x_0) = \int_{-\infty}^{\infty} \delta(x_0 - x)f(x)dx = (\delta(x)) * (f(x))$$

$$f(x_0) = \int_{-\infty}^{\infty} f(x_0 - x)\delta(x)dx = (\delta(x)) * (f(x))$$

By superposition, the response to a driving force  $f(t)$  is a sum of the impulse response functions, for our system described as  $m \frac{dv(t)}{dt} + bv(t) = f(t)$ , where we have  $\chi(t)$  as impulse response or Green’s function with  $f(t) = \delta(t)$

$$v(t) = \int_{-\infty}^{\infty} \chi(t-t')f(t')dt'$$

For a differential equation if  $\chi(t)$  is Green’s function, i.e. solution to the homogeneous equation, or solution to driving force as impulse excitation, that we call impulse response function, then to any other forcing function driving the differential equation, the solution is convolution integral with Green’s function, i.e.  $v(t) = \chi(t) * f(t) = \int_{-\infty}^{\infty} \chi(t-t')f(t')dt$ .

## 6. Fourier Transform and Conjugate Fourier Transform

In 1743 famous Swiss mathematician, Leonard Euler derived a formula i.e.

$$e^{iz} = \cos z + i \sin z$$

and about 150 years later, physicist Arthur E Kennelly and Charles P Steinmetz used the formula to introduce ‘harmonic wave forms’ in Electrical Engineering that is

$$e^{i\omega t} = \cos \omega t + i \sin \omega t; \quad e^{-i\omega t} = \cos \omega t - i \sin \omega t$$

Later on in the beginning of the 20<sup>th</sup> century, the German Scientist David Hilbert finally showed that the function  $\sin \omega t$  is the Hilbert Transform of  $\cos \omega t$ . This gave us concept of phase shift of  $\pm\pi / 2$  which is a basic property of Hilbert Transform. We note here that  $e^{i\omega t}$  has Hilbert Transform of Real Part as Imaginary part, such a function where real and imaginary parts are Hilbert Transforms of one another are called 'strong analytic functions'. We will use this Hilbert Transform in our analysis-later in this note.

A complex function  $g(t)$  has Fourier Transform as  $G(\omega)$ , where  $g(t)$  and  $G(\omega)$  are related as following integral, and are called Fourier Transformed pairs, that is  $G(\omega) = \mathcal{F}\{g(t)\}$  and  $g(t) = \mathcal{F}^{-1}\{G(\omega)\}$ .

$$G(\omega) = \int_{-\infty}^{\infty} g(t)e^{-i\omega t} dt, \quad g(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega)e^{i\omega t} d\omega$$

We have  $\bar{g}(t)$  as complex conjugate of  $g(t)$  then we have a Conjugate Fourier Transform  $\bar{G}(\omega)$  defined as following integral, we represent  $\bar{G}(\omega) = \mathcal{F}\{\bar{g}(t)\}$  and  $\bar{g}(t) = \mathcal{F}^{-1}\{\bar{G}(\omega)\}$

$$\bar{G}(\omega) = \int_{-\infty}^{\infty} \bar{g}(t)e^{i\omega t} dt, \quad \bar{g}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{G}(\omega)e^{-i\omega t} d\omega$$

Provided all the above integrals exists. For a pure real function  $g(t)$  -like impulse response function  $\chi(t)$  we have  $g(t) = \bar{g}(t)$ . So we have for a real function  $g(t)$ , we write the following

$$\begin{aligned} g(t) = \mathcal{F}^{-1}\{G(\omega)\} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega)e^{i\omega t} d\omega = \bar{g}(t); & \bar{g}(t) = \mathcal{F}^{-1}\{\bar{G}(\omega)\} &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{G}(\omega)e^{-i\omega t} d\omega \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{G}(\omega)e^{-i\omega t} d\omega; & \omega \rightarrow -\omega; & d\omega \rightarrow -d\omega \\ &= \frac{1}{2\pi} \int_{\infty}^{-\infty} \bar{G}(-\omega)e^{i\omega t} (-d\omega) \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \bar{G}(-\omega)e^{i\omega t} d\omega \end{aligned}$$

So for real function  $g(t)$  we have

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

From above we find that, for a real function  $g(t)$ , we have Fourier and Conjugate Fourier Transform related as  $G(\omega) = \bar{G}(-\omega)$  or we can also have like above steps  $G(-\omega) = \bar{G}(\omega)$ . This shows that  $G(\omega)$  for negative frequencies  $-\infty < \omega < 0$  can be expressed by conjugate Fourier Transform  $\bar{G}(\omega)$  for positive frequencies  $0 < \omega < \infty$ . Further we will show that for a real function  $g(t)$ , we get the following

$$g(t) = \frac{1}{2\pi} \int_0^{\infty} (\bar{G}(\omega)e^{-i\omega t} + G(\omega)e^{i\omega t}) d\omega$$

The proof is in following steps

$$\begin{aligned}
g(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega) e^{i\omega t} d\omega \\
&= \frac{1}{2\pi} \int_{-\infty}^0 G(\omega) e^{i\omega t} d\omega + \frac{1}{2\pi} \int_0^{\infty} G(\omega) e^{i\omega t} d\omega \\
&= \frac{1}{2\pi} \int_0^{\infty} G(-\omega) e^{-i\omega t} d\omega + \frac{1}{2\pi} \int_0^{\infty} G(\omega) e^{i\omega t} d\omega \\
&= \frac{1}{2\pi} \int_0^{\infty} \bar{G}(\omega) e^{-i\omega t} d\omega + \frac{1}{2\pi} \int_0^{\infty} G(\omega) e^{i\omega t} d\omega
\end{aligned}$$

This implies that positive frequency spectra i.e.  $0 < \omega < \infty$  with Fourier Transforms  $G(\omega)$  and its conjugate  $\bar{G}(\omega) = G(-\omega)$  is sufficient to represent a real function i.e.  $g(t)$ , by Fourier inverse formula, i.e.  $g(t) = \frac{1}{2\pi} \int_0^{\infty} (\bar{G}(\omega) e^{-i\omega t} + G(\omega) e^{i\omega t}) d\omega$ .

### 7. Inverse Fourier Transform of a Function defined only for positive frequencies gives a Complex function in time domain and its properties

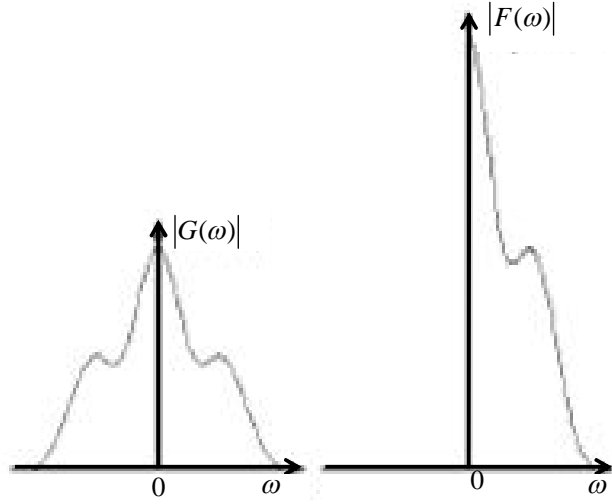
Now we see if Fourier transform that is existing only for positive frequencies ( $0 < \omega < \infty$ ) and is zero for negative frequencies, what is the nature of its Inverse Fourier Transform i.e.  $f(t) = \mathcal{F}^{-1}\{F(\omega)\}$ ? Let us define function  $F(\omega) = 0$  that is zero for all negative frequencies ( $-\infty < \omega < 0$ ) and  $F(\omega) = 2G(\omega)$  for all positive frequencies ( $0 < \omega < \infty$ )

$$\begin{aligned}
F(\omega) &= \begin{cases} 2G(\omega) & \omega \geq 0 \\ 0 & \omega < 0 \end{cases} & \text{sgn}(\omega) &= \begin{cases} 1 & , \omega > 0 \\ 0 & , \omega = 0 \\ -1 & , \omega < 0 \end{cases} \\
&= G(\omega) + (\text{sgn}(\omega))G(\omega)
\end{aligned}$$

where  $G(\omega) = \mathcal{F}\{g(t)\} = \int_{-\infty}^{\infty} g(t) e^{-i\omega t} dt$ . Refer Figure-1, we note that  $G(\omega)$  is function defined for all frequencies  $-\infty < \omega < \infty$ , while  $F(\omega)$  is defined for only positive frequencies  $0 < \omega < \infty$ . Thus we have constructed a symmetrical function (which is even function) for all frequencies from a function that is only defined for positive frequencies.



$$G(\omega) = \mathcal{F}\{g(t)\} = \int_{-\infty}^{\infty} g(t)e^{-i\omega t} dt \quad F(\omega) = G(\omega) + \text{sgn}(\omega)G(\omega)$$



**Figure-1: Amplitude of  $G(\omega)$  and  $F(\omega)$  with frequency  $\omega$**

The inverse Fourier Transform of  $F(\omega)$  is  $f(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega)e^{i\omega t} d\omega$ . Considering  $f(t)$  as complex function, i.e.  $f(t) = \text{Re}[f(t)] + i \text{Im}[f(t)] \equiv g(t) + ih(t)$ ; with  $F(\omega) = 0$  for  $\omega < 0$  constructed as  $F(\omega) = G(\omega) + (\text{sgn}(\omega))G(\omega)$  we write following steps

$$\begin{aligned} f(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega)e^{i\omega t} d\omega, \quad F(\omega) = 0, \quad \omega < 0; \quad F(\omega) = G(\omega) + \text{sgn}(\omega)G(\omega) \\ &= \frac{1}{2\pi} \int_{-\infty}^0 F(\omega)e^{i\omega t} d\omega + \frac{1}{2\pi} \int_0^{\infty} F(\omega)e^{i\omega t} d\omega; \quad F(\omega) = \begin{cases} 0, & \omega < 0 \\ 2G(\omega), & \omega > 0 \end{cases} \\ &= \frac{1}{\pi} \int_0^{\infty} G(\omega)e^{i\omega t} d\omega \\ &= \frac{1}{2\pi} \int_0^{\infty} F(\omega)e^{i\omega t} d\omega \end{aligned}$$

Where  $f(t)$  is a complex function of the form say  $f(t) = g(t) + ih(t)$ , where  $\text{Re}[f(t)] \equiv g(t)$  and  $\text{Im}[f(t)] \equiv h(t)$ . Where  $g(t)$  is real function and  $g(t) = \mathcal{F}^{-1}\{G(\omega)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega)e^{i\omega t} d\omega$ ; we are also having  $F(\omega) = G(\omega) + (\text{sgn}(\omega))G(\omega)$  as defined above. We write the following

$$\begin{aligned} f(t) &= g(t) + ih(t) = \frac{1}{\pi} \int_0^{\infty} G(\omega)e^{i\omega t} d\omega \\ f(t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} G(\omega)e^{i\omega t} d\omega + ih(t) = \frac{1}{\pi} \int_0^{\infty} G(\omega)e^{i\omega t} d\omega \end{aligned}$$

Now we will derive what is  $h(t)$  in terms of  $g(t)$  for above condition  $F(\omega) = 0$ , for  $\omega < 0$  in following steps.

$$f(t) = \mathcal{F}^{-1}\{F(\omega)\} = \frac{1}{2\pi} \int_0^{\infty} F(\omega) e^{i\omega t} d\omega; \quad F(\omega) = 0, \quad \omega < 0$$

$$f(t) = g(t) + ih(t); \quad f(t) = \frac{1}{\pi} \int_0^{\infty} G(\omega) e^{i\omega t} d\omega, \quad g(t) = \mathcal{F}^{-1}\{G(\omega)\}$$

$$F(\omega) = \mathcal{F}\{f(t)\} = \mathcal{F}\{g(t) + ih(t)\}; \quad F(\omega) = G(\omega) + (\text{sgn}(\omega)G(\omega))$$

$$F(\omega) = G(\omega) + (\text{sgn}(\omega)G(\omega)) = \mathcal{F}\{g(t)\} + \mathcal{F}\{ih(t)\}$$

We have  $G(\omega) = \mathcal{F}\{g(t)\}$ , from above we infer that  $(\text{sgn}(\omega)G(\omega)) = \mathcal{F}\{ih(t)\}$ . From the standard Fourier Tables we have  $\mathcal{F}\left\{\frac{1}{\pi t}\right\} = -i \text{sgn}(\omega)$ , with this we write the following

$$F(\omega) = G(\omega) + (\text{sgn}(\omega)G(\omega)) = \mathcal{F}\{g(t)\} + \mathcal{F}\{ih(t)\}$$

$$F(\omega) = G(\omega) + \left(-\frac{1}{i}\right)(-i \text{sgn}(\omega)G(\omega)) = \mathcal{F}\{g(t)\} + \mathcal{F}\{ih(t)\}$$

$$F(\omega) = G(\omega) + i(-i \text{sgn}(\omega)G(\omega)) = \mathcal{F}\{g(t)\} + i\mathcal{F}\{h(t)\}$$

We thus write

$$\mathcal{F}\{g(t)\} = G(\omega); \quad \mathcal{F}\{h(t)\} = (-i \text{sgn}(\omega))(G(\omega)); \quad \mathcal{F}\left\{\frac{1}{\pi t}\right\} = -i \text{sgn}(\omega)$$

$$\mathcal{F}\{g(t)\} = G(\omega); \quad \mathcal{F}\{h(t)\} = \left(\mathcal{F}\left\{\frac{1}{\pi t}\right\}\right)(\mathcal{F}\{g(t)\})$$

We have convolution theorem i.e.  $(\mathcal{F}\{f_1(t)\})(\mathcal{F}\{f_2(t)\}) = \mathcal{F}\{(f_1(t)) * (f_2(t))\}$ , and the convolution is defined as  $(f_1(t)) * (f_2(t)) = \int_{-\infty}^{\infty} f_1(t-t')f_2(t')dt'$

$$\mathcal{F}\{g(t)\} = G(\omega); \quad \mathcal{F}\{h(t)\} = \left(\mathcal{F}\left\{\frac{1}{\pi t}\right\}\right)(\mathcal{F}\{g(t)\})$$

$$f(t) = g(t) + ih(t)$$

$$g(t) = \mathcal{F}^{-1}\{G(\omega)\}; \quad h(t) = \left(\frac{1}{\pi t}\right) * (g(t)) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{g(t')}{t-t'} dt'$$

We see that  $h(t)$ , the imaginary part of the  $f(t)$  can be expressed as  $\hat{g}(t) = \mathcal{H}\{g(t)\}$  which is called Hilbert Transform of  $g(t)$ ; also we observe that  $h(t)$  is real function. We define the Hilbert Transform (we will discuss in Section-14 in detail) as following integral transform or convolution

$$\hat{g}(t) = \mathcal{H}\{g(t)\} = \left(\frac{1}{\pi t}\right) * (g(t)) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{g(t')}{t-t'} dt'$$

We will make use of this in subsequently-in deriving Kramer-Kronigs relation.

This we have analyzed for a function  $F(\omega)$  which is zero for all  $\omega < 0$ , has Fourier Inverse  $f(t) = \mathcal{F}^{-1}\{F(\omega)\}$  as complex function  $f(t) = \text{Re}[f(t)] + i \text{Im}[f(t)]$  where we have Imaginary Part as Hilbert Transform of Real Part  $\text{Im}[f(t)] = \mathcal{H}\{\text{Re}[f(t)]\}$ . This observation has implication in our

study of Causality, where we have an impulse response function  $\chi(t)$  which is zero for negative times i.e.  $t < 0$ , will have its frequency spectra as complex function  $\bar{\chi}(\omega)$ , whose real and imaginary parts are Hilbert Transforms of one another. That is what we will prove subsequently, and is called Kramer-Kronigs relation for  $\bar{\chi}(\omega)$  in order to have Causality of  $\chi(t)$ .

## 8. Response of system to harmonic field and defining susceptibility function $\bar{\chi}(\omega)$ in frequency domain

It is also practical to consider response to an applied AC field  $\bar{f}(t) = F_0 e^{-i\omega t}$  (as we do in Electrical Engineering analysis as devised by Kennelly and Steinmetz)

$$\begin{aligned} x(t) &= \int_{-\infty}^{\infty} dt' \chi(t-t') \bar{f}(t'), & \bar{f}(t) &= F_0 e^{-i\omega t} \\ x(t) &= \int_{-\infty}^{\infty} dt' \chi(t-t') F_0 e^{-i\omega t'} \end{aligned}$$

Let  $t-t' = \tau$  then we write the following

$$\begin{aligned} x(t) &= F_0 \int_{\infty}^{-\infty} (-d\tau) \chi(\tau) e^{-i\omega t} e^{i\omega\tau} \\ &= \left( \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{i\omega\tau} \right) (F_0 e^{-i\omega t}) \end{aligned}$$

But the causality implies that  $\chi(\tau) = 0$  for  $\tau < 0$ , thus we write from above

$$x(t) = \left( \int_0^{\infty} d\tau \chi(\tau) e^{i\omega\tau} \right) (F_0 e^{-i\omega t})$$

Define  $\bar{\chi}(\omega) = \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{i\omega\tau} = \int_0^{\infty} d\tau \chi(\tau) e^{i\omega\tau}$ , call it Dynamic Response Function. That is now  $\bar{\chi}(\omega)$  is a frequency dependent quantity, or frequency domain representation of the impulse response  $\chi(t)$ . This  $\bar{\chi}(\omega)$  is also called linear response coefficient or response function or dynamic susceptibility of a system. We note that  $\bar{\chi}(\omega) = \bar{\mathcal{F}}\{\chi(t)\}$  i.e. conjugate Fourier Transformed of  $\chi(t) = \bar{\chi}(t)$  which is real function.

We take complex conjugate of earlier AC field  $\bar{f}(t) = F_0 e^{-i\omega t}$  i.e.  $f(t) = F_0 e^{i\omega t}$ . With this AC field (i.e. complex conjugate of the earlier one) we get the following

$$\begin{aligned} x(t) &= \int_{-\infty}^{\infty} dt' \chi(t-t') f(t'), & f(t) &= F_0 e^{i\omega t} \\ x(t) &= \int_{-\infty}^{\infty} dt' \chi(t-t') F_0 e^{i\omega t'}, & t-t' &= \tau \\ x(t) &= F_0 \int_{\infty}^{-\infty} (-d\tau) \chi(\tau) e^{-i\omega t} e^{i\omega\tau} \\ &= \left( \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{-i\omega\tau} \right) (F_0 e^{i\omega t}) = \left( \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{-i\omega\tau} \right) (f(t)) \end{aligned}$$

We notice that in this case  $\chi(\omega) = \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{-i\omega\tau}$  is Fourier Transform of  $\chi(t)$ , the impulse response function  $\chi(\omega) = \mathcal{F}\{\chi(t)\}$ , where  $\chi(t) = 0$  for  $t < 0$ . This we got for forcing function  $f(t) = F_0 e^{i\omega t}$ , a complex conjugate of earlier function  $\bar{f}(t) = F_0 e^{-i\omega t}$ .

We point out that for  $f(t) = F_0 e^{i\omega t}$  we got  $\chi(\omega) = \int_{-\infty}^{\infty} d\tau \chi(\tau) e^{-i\omega\tau} = \mathcal{F}\{\chi(t)\}$ . This  $\chi(\omega)$  is complex conjugate of  $\bar{\chi}(\omega)$  that we obtained for  $\bar{f}(t) = F_0 e^{-i\omega t}$ . Therefore from impulse response function  $\chi(t)$  for a system, one can do Fourier Transform, and get susceptibility function  $\chi(\omega)$ , for a system excited with  $f(t) = F_0 e^{i\omega t}$ . For a system excited by  $\bar{f}(t) = F_0 e^{-i\omega t}$ , one should get Fourier Transform of impulse response function to write  $\chi(\omega)$  first and then make  $\omega \equiv -\omega$  to get  $\bar{\chi}(\omega)$ .

Say  $\chi(t) = K e^{-t/\tau}$ , for  $t \geq 0$  then for a system with AC Field excitation as  $f(t) = F_0 e^{i\omega t}$  we would write

$$\chi(\omega) = \mathcal{F}\{K e^{-t/\tau}\} = \frac{K\tau}{1+i\omega\tau} = \frac{K\tau}{1+\omega^2\tau^2} - i \frac{K\omega\tau^2}{1+\omega^2\tau^2}$$

For a system with AC field excitation as  $\bar{f}(t) = F_0 e^{-i\omega t}$  we have complex conjugate of  $\bar{\chi}(\omega)$  i.e.

$$\bar{\chi}(\omega) = \mathcal{F}\{K e^{-t/\tau}\} \Big|_{\omega \rightarrow -\omega} = \frac{K\tau}{1-i\omega\tau} = \frac{K\tau}{1+\omega^2\tau^2} + i \frac{K\omega\tau^2}{1+\omega^2\tau^2}$$

We will stick to excitation field as  $\bar{f}(t) = F_0 e^{-i\omega t}$  and develop the concepts further-in this note. We note here for  $\bar{f}(t) = F_0 e^{-i\omega t}$ , the susceptibility  $\bar{\chi}(\omega) = \int_0^{\infty} d\tau \chi(\tau) e^{i\omega\tau}$  this comes since we have  $\chi(t) = 0$  for  $t < 0$ , and for real function we have  $\chi(t) = \bar{\chi}(t)$ .

We write the following definition

$$\bar{\chi}(\omega) = \text{Re}[\bar{\chi}(\omega)] + i \text{Im}[\bar{\chi}(\omega)] = \int_0^{\infty} d\tau \chi(\tau) e^{i\omega\tau}$$

With this substitution we write for  $x(t) = \left( \int_0^{\infty} d\tau \chi(\tau) e^{i\omega\tau} \right) (F_0 e^{-i\omega t})$  the following

$$\begin{aligned} x(t) &= \bar{\chi}(\omega) F_0 e^{-i\omega t} \\ &= (\text{Re}[\bar{\chi}(\omega)] + i \text{Im}[\bar{\chi}(\omega)]) F_0 e^{-i\omega t} \end{aligned}$$

Thus dynamic susceptibility  $\bar{\chi}(\omega)$  is a complex function. Any applied input field  $f(t)$  is a 'real' quantity. So we have to interpret.

## 9. Interpretation of Complex input field

We have input field as following

$$\bar{f}(t) = F_0 e^{-i\omega t} = F_0 \cos \omega t - i F_0 \sin \omega t$$

only the ‘real-part’  $F_0 \cos \omega t$  is meant-in above complex harmonic input  $F_0 e^{-i\omega t}$ ; that takes part in excitation force. We expand as follows

$$\begin{aligned} x(t) &= \bar{\chi}(\omega) F_0 e^{-i\omega t} \\ &= (\text{Re}[\bar{\chi}(\omega)] + i \text{Im}[\bar{\chi}(\omega)])(F_0 \cos \omega t - i F_0 \sin \omega t) \\ &= (\text{Re}[\bar{\chi}(\omega)] F_0 \cos \omega t + \text{Im}[\bar{\chi}(\omega)] F_0 \sin \omega t) + i(\text{Im}[\bar{\chi}(\omega)] F_0 \cos \omega t - \text{Re}[\bar{\chi}(\omega)] F_0 \sin \omega t) \end{aligned}$$

Because the response is linear, and taking the real part of the above linear operation, to the real part of the complex field  $F_0 \cos \omega t$  is the real part of the response to the complex input field described above. This is expressed below as correct interpretation of  $x(t) = \bar{\chi}(\omega) F_0 e^{-i\omega t}$

$$\begin{aligned} x(t) &= \text{Re}[\bar{\chi}(\omega) F_0 e^{-i\omega t}] \\ &= \text{Re}[\bar{\chi}(\omega)] F_0 \cos \omega t + \text{Im}[\bar{\chi}(\omega)] F_0 \sin \omega t \end{aligned}$$

Therefore the ‘real’ and ‘imaginary’ parts of  $\bar{\chi}(\omega)$  i.e.  $\text{Re}[\bar{\chi}(\omega)]$  and  $\text{Im}[\bar{\chi}(\omega)]$  have meaning. The real part  $\text{Re}[\bar{\chi}(\omega)]$  gives the ‘in-phase’ part of the response and it oscillates like  $\cos \omega t$ , we call it ‘dissipative-part’; while the imaginary part  $\text{Im}[\bar{\chi}(\omega)]$  gives the ‘out-of-phase’ response-we term as ‘reactive response’-  $\text{Im}[\bar{\chi}(\omega)] F_0 \sin \omega t$ .

### 10. Causality is Analyticity of Dynamic Response function or Dynamic Susceptibility function $\bar{\chi}(\omega^*)$ in upper-half of complex frequency $\omega^* \equiv \text{Re}[\omega^*] + i \text{Im}[\omega^*]$ plane

The causality gives important relation between the ‘real-part’ i.e.  $\text{Re}[\bar{\chi}(\omega)]$  and ‘imaginary-part’ i.e.  $\text{Im}[\bar{\chi}(\omega)]$  of the linear response coefficient of the system  $\bar{\chi}(\omega)$ . We first show that causality implies that linear response coefficient  $\bar{\chi}(\omega^*)$  given as  $\bar{\chi}(\omega^*) = \text{Re}[\bar{\chi}(\omega^*)] + i \text{Im}[\bar{\chi}(\omega^*)] = \int_0^\infty d\tau \chi(\tau) e^{i\omega^* \tau}$  for a Real Causal time function  $\chi(t)$  is analytic in the upper-half of the complex plane  $z \equiv \omega^*$ , when  $\bar{\chi}(z)$  considered function of a complex frequency,  $z = x + iy \equiv \omega^*$ . Here we note that  $\text{Re}[z] = x \equiv \omega$  is the physical frequency  $\omega$  that we had been discussing in previous section. So the  $\bar{\chi}(z)$  is

$$\begin{aligned} \bar{\chi}(z) &= \text{Re}[\bar{\chi}(z)] + i \text{Im}[\bar{\chi}(z)] = \int_0^\infty d\tau \chi(\tau) e^{i(x+iy)\tau} \\ &= \int_0^\infty d\tau \chi(\tau) e^{-y\tau} \cos(x\tau) + i \int_0^\infty d\tau \chi(\tau) e^{-y\tau} \sin(x\tau) \end{aligned}$$

From above we write following

$$\text{Re}[\bar{\chi}(z)] = \int_0^\infty d\tau \chi(\tau) e^{-y\tau} \cos(x\tau) \quad \text{Im}[\bar{\chi}(z)] = \int_0^\infty d\tau \chi(\tau) e^{-y\tau} \sin(x\tau)$$

We note that  $\text{Re}[\bar{\chi}(z)]$  is even function in variable  $x$  (or  $\omega$  the physical frequency), and  $\text{Im}[\bar{\chi}(z)]$  is odd function in variable  $x$  (or  $\omega$  the physical frequency).

Sufficient condition of analyticity is via Cauchy-Riemann equation. That is for  $\bar{\chi}(z)$  a complex function of complex variable  $z = x + iy$  to be analytic the condition is following

$$\frac{\partial}{\partial x} \operatorname{Re}[\bar{\chi}(x + iy)] = \frac{\partial}{\partial y} \operatorname{Im}[\bar{\chi}(x + iy)] \quad \frac{\partial}{\partial x} \operatorname{Im}[\bar{\chi}(x + iy)] = -\frac{\partial}{\partial y} \operatorname{Re}[\bar{\chi}(x + iy)]$$

We apply this above Cauchy-Riemann relation and see the following

$$\begin{aligned} \frac{\partial}{\partial x} \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} \cos(x\tau) &= \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} (-\tau \sin(x\tau)) \\ \frac{\partial}{\partial y} \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} \sin(x\tau) &= \int_0^{\infty} d\tau \chi(\tau) (-\tau e^{-y\tau}) \sin(x\tau) \\ \frac{\partial}{\partial x} \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} \sin(x\tau) &= \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} (\tau \cos(x\tau)) \\ \frac{\partial}{\partial y} \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} \cos(x\tau) &= \int_0^{\infty} d\tau \chi(\tau) (-\tau e^{-y\tau}) \cos(x\tau) \end{aligned}$$

We see the Cauchy-Riemann condition is satisfied. Hence we can say  $\bar{\chi}(x + iy) \equiv \bar{\chi}(\omega^*)$  is analytic.

But what we did in the above steps is that we interchanged the derivative and integration operators. This is only possible if the integrals that are representing  $\operatorname{Re}[\bar{\chi}(z)] = \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} \cos(x\tau)$  and

$\operatorname{Im}[\bar{\chi}(z)] = \int_0^{\infty} d\tau \chi(\tau) e^{-y\tau} \sin(x\tau)$  are ‘absolutely convergent’. This property of absolute convergent holds true for  $y > 0$  (for any positive  $\tau \equiv t - t'$  which is must for causality  $\tau > 0$ ). The integrands are therefore a type of damped oscillatory function, multiplied by  $\chi(\tau)$  (that is also a decaying type function as we discussed previously) and this integral will be finite (convergent). We have seen  $\tau \equiv t - t'$  is positive, as the observation time for response of ‘effect’  $\chi(\tau)$  i.e. with  $t$  is always greater than application time of force (cause) i.e.  $t'$ , i.e.  $t > t'$ , is Causality.

We note that the absolute convergent condition of the integrals would not be there for case  $\tau < 0$  - with  $\chi(\tau) \neq 0$  meaning  $t < t'$  implying effect  $\chi(\tau)$  is observed before application of cause; that is for system which is non-Causal. Thus for  $y > 0$  i.e. in the upper half of the complex plane  $z$ , we will be having diverging integrals in form of un-damped and growing oscillatory functions in the integral. Thus in the Cauchy-Riemann tests we will be not able to interchange the derivative and integration operation, so the relations will fail. In that case for non-Causal where  $\tau < 0$  and  $\chi(\tau) \neq 0$  we will not have analyticity of  $\bar{\chi}(z)$  in the upper-half of the complex plane. Thus for non-Causal case analyticity is lost.

## 11. Titchmarsh's Theorem

The theorem states that the following conditions for a complex-valued square-integrable function  $f: \mathbb{R} \rightarrow \mathbb{C}$  are equivalent:

$f(x)$  is the limit as  $z \equiv (x + iy) \rightarrow x$  of a holomorphic (analytic) function  $f(z)$  in the upper half-plane

i.e. ( $y > 0$ ) such that  $\int_{-\infty}^{\infty} |f(x + iy)|^2 dx < K$ , for some number  $K$  and  $y > 0$  (i.e. the integral is bounded).

The real and imaginary parts of  $f(x)$  are Hilbert transforms (that we will describe shortly) of each other.

The Fourier transform  $\mathcal{F}\{f(x)\} = F(k)$  vanishes for  $k < 0$ .

In our application therefore the condition  $y > 0$  is the zone in ‘upper-half’ of  $z$  plane; (the complex frequency plane  $\omega^*$ ). This means  $\bar{\chi}(z) = \int_0^\infty d\tau \chi(\tau) e^{iz\tau}$  is analytic in ‘upper half of complex’ plane for  $\chi(\tau)$  to be causal. This conclusion is called Titchmarsh’s theorem (1948). This extends to the real frequency axis we call  $\omega$  i.e.  $\text{Re}[z] = x \equiv \omega$  only if we add the condition that is  $\lim_{\tau \uparrow \infty} \chi(\tau) = 0$ , which sometimes is true and sometimes not true in physical applications. It is also clear that if  $\chi(\tau)$  had not been causal, meaning  $\chi(\tau) \neq 0$  for  $\tau < 0$  as well as  $\tau > 0$ , then analyticity would not have been established anywhere.

The fact that the upper rather than the lower half of the complex plane where  $\bar{\chi}(z)$  is analytic follows from the arbitrary sign in input field  $\bar{f}(t) = F_0 e^{-i\omega t}$ , i.e. input field oscillates as  $e^{-i\omega t}$  rather than  $e^{+i\omega t}$ . These choices are equally fine, so it is necessary to choose a convention and stick to it.

## 12. Applying Cauchy’s Integral Formula to Analytic Dynamic Response Function $\bar{\chi}(z)$ for Causal $\chi(t)$

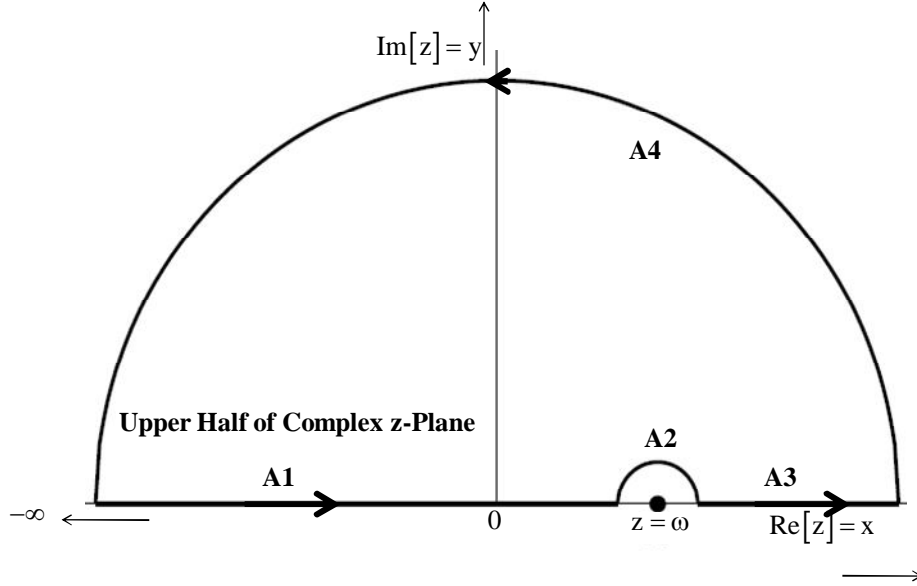
Thus if complex function  $\bar{\chi}(z)$  is analytic in and on a closed contour  $C$  in the complex plane  $z$ ; then the condition i.e.  $\int_C \bar{\chi}(z) dz = 0$  holds. Cauchy’s integral formula allows us to write the following

$$\bar{\chi}(\omega) = \frac{1}{2\pi i} \int_C \frac{\bar{\chi}(z) dz}{z - \omega}$$

In the above Cauchy’s integral formula  $\omega$  is any point on ‘upper half’  $z$  plane (where due to Causality of  $\chi(t)$ , complex function  $\bar{\chi}(z)$  is analytic), and  $C$  is any closed contour containing  $\omega$  lying entirely within upper half plane or on the real axis (if analyticity extends that far). The integration on contour is anti-clockwise direction as shown by arrows in Figure-1. We note that  $z = \omega$  is a pole in complex function integrand. If the contour does not contain the pole  $z = \omega$ , then we have the above integral on closed contour as zero.

$$0 = \int_C \frac{\bar{\chi}(z) dz}{z - \omega}$$

We draw the contour as in Figure-2. The contour  $C$  is having parts (i) A1 a straight line from  $-\infty$  to the left edge of the semi-circle A2 encircling the point  $z = \omega$ , (ii) the semicircle A2, (iii) the straight line A3 from right edge of semicircle to  $+\infty$ , (iv) the big arc of semicircle with infinite radius A4. Therefore we have  $C = A1 \cup A2 \cup A3 \cup A4$ , a closed contour on real axis extending to upper half plane, and not enclosing the singular point i.e.  $z = \omega$ .



**Figure-2: Showing contour of integration in upper half plane**

We have shown that  $\bar{\chi}(z)$  is analytic in the upper half plane i.e.  $\text{Im}[z] = y > 0$ , for  $\chi(t)$  to be causal, and with condition that  $\lim_{|z| \rightarrow \infty} \bar{\chi}(z) = 0$  (i.e. adding Titchmarsh's condition); we draw the closed contour C depicted in Figure-2. The integration is thus

$$\int_C \frac{\bar{\chi}(z) dz}{z - \omega} = \int_{A1} \frac{\bar{\chi}(z) dz}{z - \omega} + \int_{A2} \frac{\bar{\chi}(z) dz}{z - \omega} + \int_{A3} \frac{\bar{\chi}(z) dz}{z - \omega} + \int_{A4} \frac{\bar{\chi}(z) dz}{z - \omega} = 0$$

The contour C is confined to the region where  $\bar{\chi}(z)$  is analytic, and does not contain the point  $z = \omega$ . Because of the condition i.e.  $\bar{\chi}(z)$  vanishes as  $|z|$  goes to infinity, the large arc of C i.e. part A4 contributes nothing to the above integral. So the only contribution is thus from A1, A2 and A3. While the semicircle A2 becomes smaller and smaller when we make its radius tending to zero, we write the integral on A1 plus integral on A2 becomes Principal Value Integral and we call that as  $\int_{-\infty}^{+\infty} \frac{\bar{\chi}(z) dz}{z - \omega}$ . We represent A2 as  $re^{i\theta} + \omega$  with  $r$  tending to zero and  $\theta$  varying from  $\pi$  to 0.

$$\begin{aligned} \int_C \frac{\bar{\chi}(z) dz}{z - \omega} &= \int_{A1} \frac{\bar{\chi}(z) dz}{z - \omega} + \int_{A2} \frac{\bar{\chi}(z) dz}{z - \omega} + \int_{A3} \frac{\bar{\chi}(z) dz}{z - \omega} = 0 \\ \int_{A1} \frac{\bar{\chi}(z) dz}{z - \omega} + \int_{A3} \frac{\bar{\chi}(z) dz}{z - \omega} + \lim_{r \downarrow 0} \int_{z=re^{i\theta}} \frac{\bar{\chi}(z) dz}{z - \omega} &= 0 \\ \int_{-\infty}^{+\infty} \frac{\bar{\chi}(z) dz}{z - \omega} + \lim_{r \downarrow 0} \int_{z=\omega+re^{i\theta}} \frac{\bar{\chi}(z) dz}{z - \omega} &= 0 \end{aligned}$$

We continue in following steps



$$\int_{-\infty}^{+\infty} \frac{\bar{\chi}(z)dz}{z-\omega} + \lim_{r \downarrow 0} \int_{\pi}^0 ire^{i\theta} d\theta \frac{\bar{\chi}(\omega + re^{i\theta})}{re^{i\theta}} = 0$$

$$\int_{-\infty}^{+\infty} \frac{\bar{\chi}(z)dz}{z-\omega} - i\pi\bar{\chi}(\omega) = 0$$

From above we write, by changing the complex variable  $z$  to  $\omega'$  a general expression as

$$\bar{\chi}(\omega) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\bar{\chi}(\omega')}{\omega' - \omega}$$

In the above derivation, we have made  $\int_{A1} \frac{\bar{\chi}(z)dz}{z-\omega} + \int_{A3} \frac{\bar{\chi}(z)dz}{z-\omega} \equiv \int_{-\infty}^{+\infty} \frac{\bar{\chi}(z)dz}{z-\omega}$ , as in the contour A2 is infinitesimal small semicircle. Thus  $\int_{-\infty}^{+\infty} \frac{\bar{\chi}(\omega')}{\omega' - \omega} d\omega'$ , the improper integral in the formula derived should be understood in 'Principal Value' sense.

### 13. Deriving Kramer-Kronigs relation in Frequency Domain

We can further write as following separating real and imaginary parts of  $\bar{\chi}(\omega)$  as

$$\bar{\chi}(\omega) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\bar{\chi}(\omega')}{\omega' - \omega}, \quad \bar{\chi}(\omega) = \text{Re}[\bar{\chi}(\omega)] + i \text{Im}[\bar{\chi}(\omega)]$$

$$\text{Re}[\bar{\chi}(\omega)] + i \text{Im}[\bar{\chi}(\omega)] = \frac{1}{i\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega' - \omega} + \frac{1}{i\pi} \int_{-\infty}^{+\infty} d\omega' \frac{i \text{Im}[\bar{\chi}(\omega')]}{\omega' - \omega}$$

$$= \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} - i \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega' - \omega}$$

This gives the following relations called Kramer-Kronigs relation in frequency domain. This Kramer-Kronigs relation relates Real part and Imaginary Part of Dynamic Response Function or Dynamic Susceptibility Function  $\bar{\chi}(\omega)$

$$\text{Re}[\bar{\chi}(\omega)] = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} \quad \text{Im}[\bar{\chi}(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega' - \omega}$$

We do the following simplification, with observation that  $\text{Im}[\bar{\chi}(x)]$  is odd function in  $x$ , that is  $\text{Im}[\bar{\chi}(-\omega)] = -\text{Im}[\bar{\chi}(\omega)]$

$$\begin{aligned}
\operatorname{Re}[\bar{\chi}(\omega)] &= \frac{1}{\pi} \int_{-\infty}^{+\infty} dx \frac{\operatorname{Im}[\bar{\chi}(x)]}{x - \omega} = \frac{1}{\pi} \int_{-\infty}^0 dx \frac{\operatorname{Im}[\bar{\chi}(x)]}{x - \omega} + \frac{1}{\pi} \int_0^{+\infty} dx \frac{\operatorname{Im}[\bar{\chi}(x)]}{x - \omega} \\
&= \frac{1}{\pi} \int_{-\infty}^0 d(-\omega') \frac{\operatorname{Im}[\bar{\chi}(-\omega')]}{(-\omega') - \omega} \Big|_{x=-\omega'} + \frac{1}{\pi} \int_0^{+\infty} d\omega' \frac{\operatorname{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} \Big|_{x=\omega'} \\
&= -\frac{1}{\pi} \int_{-\infty}^0 d(\omega') \frac{(-\operatorname{Im}[\bar{\chi}(\omega')])}{(\omega' + \omega)} + \frac{1}{\pi} \int_0^{+\infty} d\omega' \frac{\operatorname{Im}[\bar{\chi}(\omega')]}{\omega' - \omega}, \quad \operatorname{Im}[\bar{\chi}(-\omega')] = -\operatorname{Im}[\bar{\chi}(\omega')] \\
&= \frac{1}{\pi} \int_0^{\infty} d\omega' \frac{\operatorname{Im}[\bar{\chi}(\omega')]}{\omega' + \omega} + \frac{1}{\pi} \int_0^{+\infty} d\omega' \frac{\operatorname{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} \\
&= \frac{2}{\pi} \int_0^{\infty} d\omega' \frac{\omega' \operatorname{Im}[\bar{\chi}(\omega')]}{\omega'^2 - \omega^2}
\end{aligned}$$

We do the following simplification, with observation that  $\operatorname{Re}[\bar{\chi}(x)]$  is even function in  $x$ , that is  $\operatorname{Re}[\bar{\chi}(-\omega)] = \operatorname{Re}[\bar{\chi}(\omega)]$

$$\begin{aligned}
\operatorname{Im}[\bar{\chi}(\omega)] &= -\frac{1}{\pi} \int_{-\infty}^{+\infty} dx \frac{\operatorname{Re}[\bar{\chi}(x)]}{x - \omega} = -\left( \frac{1}{\pi} \int_{-\infty}^0 dx \frac{\operatorname{Re}[\bar{\chi}(x)]}{x - \omega} + \frac{1}{\pi} \int_0^{+\infty} dx \frac{\operatorname{Re}[\bar{\chi}(x)]}{x - \omega} \right) \\
&= -\left( \frac{1}{\pi} \int_{-\infty}^0 d(-\omega') \frac{\operatorname{Re}[\bar{\chi}(-\omega')]}{(-\omega') - \omega} \Big|_{x=-\omega'} + \frac{1}{\pi} \int_0^{+\infty} d\omega' \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{\omega' - \omega} \Big|_{x=\omega'} \right) \\
&= -\left( -\frac{1}{\pi} \int_{-\infty}^0 d(-\omega') \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{(\omega' + \omega)} + \frac{1}{\pi} \int_0^{+\infty} d\omega' \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{\omega' - \omega} \right); \quad \operatorname{Re}[\bar{\chi}(-\omega')] = \operatorname{Re}[\bar{\chi}(\omega')] \\
&= -\left( -\frac{1}{\pi} \int_0^{\infty} d\omega' \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{\omega' + \omega} + \frac{1}{\pi} \int_0^{+\infty} d\omega' \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{\omega' - \omega} \right) \\
&= -\frac{2\omega}{\pi} \int_0^{\infty} d\omega' \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{\omega'^2 - \omega^2}
\end{aligned}$$

We have derived Kramer-Kronigs relation for  $\operatorname{Re}[\bar{\chi}(\omega)]$  and  $\operatorname{Im}[\bar{\chi}(\omega)]$  for frequencies  $-\infty < \omega < \infty$  and above we have derived Kramer-Kronigs relation, in frequency domain for relating real and imaginary parts of susceptibility function  $\operatorname{Re}[\bar{\chi}(\omega)]$  and  $\operatorname{Im}[\bar{\chi}(\omega)]$  for  $0 < \omega < \infty$ . That is

$$\operatorname{Re}[\bar{\chi}(\omega)] = \frac{2}{\pi} \int_0^{\infty} d\omega' \frac{\omega' \operatorname{Im}[\bar{\chi}(\omega')]}{\omega'^2 - \omega^2}; \quad \operatorname{Im}[\bar{\chi}(\omega)] = -\frac{2\omega}{\pi} \int_0^{\infty} d\omega' \frac{\operatorname{Re}[\bar{\chi}(\omega')]}{\omega'^2 - \omega^2}$$

#### 14. Hilbert transforms a review

Here we will describe briefly about Hilbert Transforms, that we have introduced in the earlier section, of Fourier Transforms. The Hilbert Transform  $\hat{f}(t)$  of a function  $f(t)$  defined for all  $t$  is described by, following integral, if the integral exists

$$\hat{f}(t) = \frac{1}{\pi} \text{P.V.} \int_{-\infty}^{\infty} \frac{f(\tau) d\tau}{t - \tau}$$

The  $\hat{f}(t) = \mathcal{H}\{f(t)\}$  is another way of writing Hilbert Transform of  $f(t)$ . We state again that Hilbert Transform is convolution of two functions

$$\hat{f}(t) = \mathcal{H}\{f(t)\} = k_c(t) * f(t) = \left(\frac{1}{\pi t}\right) * f(t)$$

That is described by above integral. The kernel of integration  $\frac{1}{\pi t}$  is also called Cauchy kernel  $k_c(t)$ . The above integral  $\int_{-\infty}^{\infty} \frac{f(\tau) d\tau}{t - \tau}$  is not possible to calculate, because of pole at  $\tau = t$ . Thus in front of the integral P.V indicates Cauchy's Principal value. We used this Cauchy's Principal Value in derivation of  $\bar{\chi}(\omega) = \frac{1}{i\pi} \int_{-\infty}^{+\infty} \frac{\bar{\chi}(\omega')}{\omega' - \omega} d\omega'$  in the previous section-where we applied Cauchy's Integral formula.

As we have stated earlier the Hilbert Transformation is phase shift operation by  $\pm\pi/2$ , we describe this concept. The phase shift of  $\pm\pi/2$  operation in frequency domain  $\omega$  is a multiplication with imaginary number i.e.  $\pm i$ . Thus we call  $K_c(\omega)$  as phase shift operator in frequency domain, that is described as

$$K_c(\omega) \stackrel{\text{def}}{=} \begin{cases} -i = e^{-i\pi/2}; & \omega > 0 \\ +i = e^{+i\pi/2}; & \omega < 0 \end{cases}$$

We will show that inverse Fourier Transform of the phase shift operator  $K_c(\omega)$  is the Cauchy kernel  $k_c(t) = \frac{1}{\pi t}$ . The  $K_c(\omega) = \mathcal{F}\{k_c(t)\}$  is not a property of Fourier Transform, yet the above can be tackled by expressing  $K_c(\omega)$  in a limit of a bounded function say  $\mathcal{G}(\omega)$ , that is

$$\lim_{\epsilon \downarrow 0} \mathcal{G}(\omega) = K_c(\omega) = \begin{cases} -i = e^{-i\pi/2}; & \omega > 0 \\ +i = e^{+i\pi/2}; & \omega < 0 \end{cases} \quad \mathcal{G}(\omega) = \begin{cases} -ie^{-\epsilon\omega}; & \omega > 0 \\ +ie^{+\epsilon\omega}; & \omega < 0 \end{cases}$$

We now apply formula for inverse Fourier Transform to  $\mathcal{G}(\omega)$  and get  $g(t)$  as below

$$\begin{aligned} g(t) &= \mathcal{F}^{-1}\{\mathcal{G}(\omega)\} \\ &= \frac{1}{2\pi} \int_{-\infty}^0 (ie^{\epsilon\omega}) e^{i\omega t} d\omega + \frac{1}{2\pi} \int_0^{\infty} (-ie^{-\epsilon\omega}) e^{i\omega t} d\omega \\ &= \frac{1}{2\pi} \int_{\infty}^0 (ie^{-\epsilon\omega}) e^{-i\omega t} (-d\omega) + \frac{1}{2\pi} \int_0^{\infty} (-ie^{-\epsilon\omega}) e^{i\omega t} d\omega \\ &= \frac{i}{2\pi} \int_0^{\infty} (e^{-(\epsilon+it)\omega} - e^{-(\epsilon-it)\omega}) d\omega = \frac{i}{2\pi} \left[ -\frac{e^{-(\epsilon+it)\omega}}{(\epsilon+it)} + \frac{e^{-(\epsilon-it)\omega}}{(\epsilon-it)} \right]_{\omega=0}^{\omega=\infty} \\ &= \frac{t}{\pi(\epsilon+t^2)} \end{aligned}$$

Now we get by inverse Fourier transform of 'impulse response' or the phase shift operator  $k_c(t) = \mathcal{F}^{-1}\{K_c(\omega)\}$  as follows

$$k_c(t) = \lim_{\epsilon \downarrow 0} g(t) = \lim_{\epsilon \downarrow 0} \frac{t}{\pi(\epsilon^2 + t^2)}$$

$$k_c(t) = \frac{1}{\pi t}$$

A convolution of  $f(t)$  and Cauchy kernel (impulse response) function  $k_c(t)$  gives Hilbert transform

$$\hat{f}(t) = k_c(t) * f(t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(\tau)}{t - \tau} d\tau$$

The Hilbert transform is used to create analytic signal function in complex plane from a real function. Instead of studying the function in transformed frequency domain  $\omega$  it is possible to view at a rotating phase vector with instantaneous phase  $\varphi(t)$  and instantaneous amplitude  $A(t)$  in time domain, for analytic function in time domain constructed as

$$g(t) = f(t) + i\hat{f}(t) = A(t)e^{i\varphi(t)}$$

Where the imaginary part is Hilbert Transform of the Real part, for the complex function  $g(t)$ , where  $f(t)$  and  $\hat{f}(t)$  are real functions of time. The above is polar form notation and we write instantaneous amplitude and phase angle as following

$$A(t) = \sqrt{f^2(t) + \hat{f}^2(t)} \quad \varphi(t) = \tan^{-1}\left(\frac{\hat{f}(t)}{f(t)}\right)$$

Assuming instantaneous phase function  $\varphi(t)$  is analytic at  $t = t_0$ , that has Taylor series, we write as

$$\varphi(t) = \varphi(t_0) + (t - t_0)\varphi^{(1)}(t_0) + \text{Rem}$$

Where  $\text{Rem}$  is remainder term with all higher derivatives, we consider to be very small when  $t \rightarrow t_0$ . Thus the analytic constructed function becomes following

$$\begin{aligned} g(t) &= f(t) + i\hat{f}(t) \\ &= A(t)e^{i\varphi(t)} = A(t)e^{i(\varphi(t_0) + (t - t_0)\varphi^{(1)}(t_0) + \text{Rem})} \\ &= A(t)e^{i(\varphi(t_0) - t_0\varphi^{(1)}(t_0))} e^{it\varphi^{(1)}(t_0)} e^{i(\text{Rem})} \end{aligned}$$

Thus for small  $\text{Rem}$  at  $t \approx t_0$  we get the following

$$g(t) = A(t)e^{i(\varphi(t_0) - t_0\varphi^{(1)}(t_0))} e^{it\varphi^{(1)}(t_0)}$$

We introduce above the notion of instantaneous frequency for  $\varphi^{(1)}(t_0)$  as  $\omega(t)$

$$\omega(t) = \frac{d\varphi(t)}{dt}$$

Take for example  $f(t) = \cos \omega_0 t$ , then we have  $\hat{f}(t) = \sin \omega_0 t$ , together they form analytic function in time  $g(t) = f(t) + i\hat{f}(t) = \cos \omega_0 t + i \sin \omega_0 t$ , with instantaneous amplitude as  $A(t) = 1$  and instantaneous phase  $\varphi(t) = \omega_0 t$ , i.e.

$$g(t) = \cos \omega_0 t + i \sin \omega_0 t = e^{i\omega_0 t} = e^{i\varphi(t)}$$

From here the instantaneous frequency is  $\omega(t) = \frac{d}{dt} \varphi(t) = \omega_0$ , which is same as real frequency, in this particular case.

### 15. Real and Imaginary Part of the Complex Susceptibility (Dynamic Response Function) $\bar{\chi}(\omega)$ are Hilbert Transforms of each other for Causal System with impulse response in time as $\chi(t)$

The basic derived relation from Cauchy's Integration formula for analytic function  $\bar{\chi}(\omega^*)$  in upper half plane of complex plane  $\omega^*$  for a Causal  $\chi(t)$  is Kramer-Kronig relation, as follows

$$\text{Re}[\bar{\chi}(\omega)] = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} \quad \text{Im}[\bar{\chi}(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega' - \omega}$$

We write Hilbert Transform formula as  $\mathcal{H}\{f(x)\}$  following  $\mathcal{H}\{f(x)\} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{f(y)dy}{x-y}$

The above improper integral is understood as Principal Value sense that we have described during derivation of Kramer-Kronigs relation. The Hilbert Transform formula above is understood as convolution integration as  $\mathcal{H}\{f(x)\} = f(x) * k_c(x)$ , where  $k_c(x)$  is Cauchy's Kernel,  $k_c(x) = \frac{1}{\pi x}$ .

Hilbert Transform of  $f(x) = \cos ax$  for  $a > 0$  is  $\mathcal{H}\{\cos ax\} = \cos(ax - \frac{\pi}{2})$ , a simple  $90^\circ$  phase lag. Applying the Hilbert Transform formula we find the Kramer-Kronig relations are following

$$\text{Re}[\bar{\chi}(\omega)] = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} = -\mathcal{H}\{\text{Im}[\bar{\chi}(\omega')]\}$$

$$\text{Im}[\bar{\chi}(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega' - \omega} = \mathcal{H}\{\text{Re}[\bar{\chi}(\omega')]\}$$

A Causal susceptibility function or response function will be having its real part as negative of Hilbert Transform of imaginary part, and its imaginary part as Hilbert Transform of the real part-else for non-Causal systems they are not. The real part is dissipation or storage part and imaginary part is the absorbing or loss part of the susceptibility or response function in frequency domain. Thus in experimentation if we determine the losses vis-à-vis frequency for any material property, then we can determine the dissipation part (real part) by performing Hilbert Transform, as stated in the above statements of Kramer-Kronigs relation.

### 16. Composing the Causal Impulse Response Function in time domain $\chi(t)$ as non-Causal Even and Odd Functions

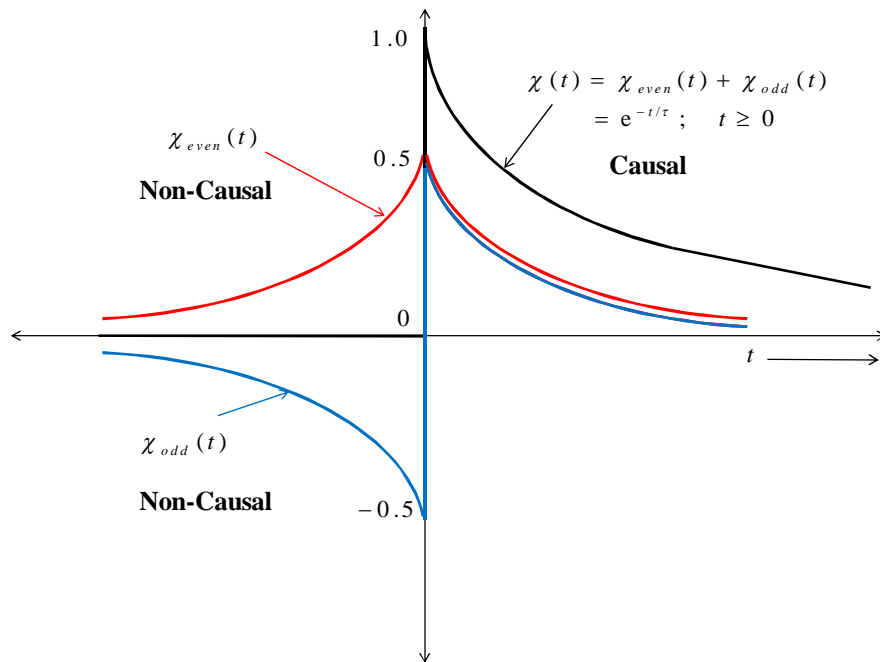
In Section-5, we constructed double sided function in frequency domain  $\omega$ , for a function  $F(\omega)$ , which is defined in positive frequencies  $0 < \omega < \infty$  and  $F(\omega) = 0$ , for negative frequencies. Then we analyzed the same and obtained inverse Fourier transform  $f(t) \equiv \text{Re}[f(t)] + i \text{Im}[f(t)]$ , and seen its properties. Here in this section we will do similar construct for a causal time domain function  $\chi(t)$ . To be of the causal

nature of the impulse response function  $\chi(t)$  (it has to be zero for  $t < 0$ ). This causality has consequences for the form of the susceptibility  $\bar{\chi}(\omega)$  that we described in frequency domain as Kramer-Kronig relations. Any function say  $\chi(t)$  can be written in terms of an even component  $\chi_{even}(t)$  and an odd component  $\chi_{odd}(t)$ . We write our impulse response function  $\chi(t)$  as following composition

$$\chi(t) = \chi_{even}(t) + \chi_{odd}(t)$$

Since the impulse response function must be zero for  $t < 0$  the even and the odd components must add to zero for  $t < 0$ . We have in our example  $m \frac{dv(t)}{dt} + bv(t) = f(t)$  we have Green's function as  $\chi(t) = \frac{1}{m} e^{-t/\tau}$ , for  $t \geq 0$  and  $\chi(t) = 0$  for  $t < 0$ . Considering  $m = 1$ , we have even and odd components for  $\chi(t)$  as

$$\chi_{even}(t) = \frac{1}{2} e^{t/\tau} \Big|_{t < 0} + \frac{1}{2} e^{-t/\tau} \Big|_{t \geq 0} \quad \chi_{odd}(t) = -\frac{1}{2} e^{t/\tau} \Big|_{t < 0} + \frac{1}{2} e^{-t/\tau} \Big|_{t \geq 0}$$



**Figure-3: Composing causal impulse response function by non-causal even and odd components**

Refer Figure-3, for the composition of causal function with non-causal functions of even and odd types. We note that in though the Green's function  $\chi(t)$  is causal, i.e. it appears as response at  $t \geq 0$ , and not for  $t < 0$ , the functions  $\chi_{even}(t)$  and  $\chi_{odd}(t)$  are non-causal, i.e. they are defined for  $t < 0$  as well as  $t \geq 0$ . By this construct as above we get  $\chi_{even}(t) + \chi_{odd}(t) = 0$  for  $t < 0$  and  $\chi_{even}(t) + \chi_{odd}(t) = e^{-t/\tau} = \chi(t)$  for  $t \geq 0$ . We note that  $\chi_{even}(t)$  is continuous at  $t = 0$ , and we have  $\chi_{even}(0^+) = \chi_{even}(0^-) = \frac{1}{2}$ , whereas

$\chi_{odd}(t)$  is discontinuous at  $t = 0$ , with  $\chi_{odd}(0^-) = -\frac{1}{2}$  and  $\chi_{odd}(0^+) = \frac{1}{2}$ . Therefore we have composed causal function in terms of anti-causal functions.

We apply  $\text{sgn}(t)$  function to  $\chi_{odd}(t)$  and  $\chi_{even}(t)$  to get the following, noting that  $\text{sgn}(t) = -1$  for  $t < 0$  and  $\text{sgn}(t) = +1$  for  $t \geq 0$ .

$$\begin{aligned} (\text{sgn}(t))(\chi_{odd}(t)) &= (\text{sgn}(t))\left(-\frac{1}{2}e^{t/\tau}\Big|_{t<0}\right) + (\text{sgn}(t))\left(\frac{1}{2}e^{-t/\tau}\Big|_{t\geq 0}\right) \\ &= \frac{1}{2}e^{t/\tau}\Big|_{t<0} + \frac{1}{2}e^{-t/\tau}\Big|_{t\geq 0} = \chi_{even}(t) \\ (\text{sgn}(t))(\chi_{even}(t)) &= (\text{sgn}(t))\left(\frac{1}{2}e^{t/\tau}\Big|_{t<0}\right) + (\text{sgn}(t))\left(\frac{1}{2}e^{-t/\tau}\Big|_{t\geq 0}\right) \\ &= -\frac{1}{2}e^{t/\tau}\Big|_{t<0} + \frac{1}{2}e^{-t/\tau}\Big|_{t\geq 0} = \chi_{odd}(t) \end{aligned}$$

Note that if we know the either the even component or the odd component of  $\chi(t)$  we construct the other, by following rule

$$\begin{aligned} \chi_{even}(t) &= (\text{sgn}(t))(\chi_{odd}(t)) = \frac{1}{2}\left(\chi(-t)\Big|_{t<0} + \chi(t)\Big|_{t\geq 0}\right) \\ \chi_{odd}(t) &= (\text{sgn}(t))(\chi_{even}(t)) = \frac{1}{2}\left(-\chi(-t)\Big|_{t<0} + \chi(t)\Big|_{t\geq 0}\right) \end{aligned}$$

## 17. Taking Fourier Transform of Even and Odd Components $\chi(t)$

We take Fourier Transform of  $\chi(t)$  and write the following for  $\chi(\omega) = \text{Re}[\chi(\omega)] + i \text{Im}[\chi(\omega)]$  the generalized susceptibility function, defined as real and imaginary parts as follows

From definition of Fourier transform we write  $\chi(\omega) = \int_{-\infty}^{\infty} \chi(t)e^{-i\omega t} dt$  and using  $\chi(t) = \chi_{even}(t) + \chi_{odd}(t)$  we have following steps

$$\begin{aligned} \chi(\omega) &= \int_{-\infty}^{\infty} \chi(t)e^{-i\omega t} dt \\ &= \int_{-\infty}^{\infty} (\chi_{even}(t) + \chi_{odd}(t))e^{-i\omega t} dt = \int_{-\infty}^{\infty} (\chi_{even}(t) + \chi_{odd}(t))(\cos \omega t - i \sin \omega t) dt \\ &= \int_{-\infty}^{\infty} \chi_{even}(t) \cos \omega t dt - i \int_{-\infty}^{\infty} \chi_{odd}(t) \sin \omega t dt = \text{Re}[\chi(\omega)] + i \text{Im}[\chi(\omega)] \end{aligned}$$

Because  $\chi_{even}(t) \sin \omega t$  is odd function and  $\int_{-\infty}^{\infty} \chi_{even}(t) \sin \omega t dt = 0$  also  $\chi_{odd}(t) \cos \omega t$  is odd function and  $\int_{-\infty}^{\infty} \chi_{odd}(t) \cos \omega t dt = 0$  these terms do not appear in above steps. Therefore we write the following

$$\operatorname{Re}[\chi(\omega)] = \int_{-\infty}^{\infty} \chi_{\text{even}}(t) \cos \omega t dt \quad \operatorname{Im}[\chi(\omega)] = -\int_{-\infty}^{\infty} \chi_{\text{odd}}(t) \sin \omega t dt$$

Moreover  $\operatorname{Re}[\chi(\omega)]$  is an even function  $\operatorname{Re}[\chi(\omega)] = \operatorname{Re}[\chi(-\omega)]$  while  $\operatorname{Im}[\chi(\omega)]$  is an odd function  $\operatorname{Im}[\chi(\omega)] = -\operatorname{Im}[\chi(-\omega)]$ .

## 18. The Kramer-Kronig relations in time domain

The Kramer-Kronig relations describe how the real and imaginary parts of the susceptibility are related to each other. If either the real part or the imaginary part of the susceptibility is known for positive frequencies  $\omega > 0$  the entire susceptibility can be calculated at all frequencies (negative as well as positive). Suppose we know  $\operatorname{Re}[\chi(\omega)]$  for  $\omega > 0$ . Then  $\operatorname{Re}[\chi(\omega)]$  for all frequencies can be constructed because  $\operatorname{Re}[\chi(\omega)] = \operatorname{Re}[\chi(-\omega)]$ . The even component of the impulse response function  $\chi_{\text{even}}(t)$  can be found by inverse Fourier ‘cosine’ transform of  $\operatorname{Re}[\chi(\omega)]$ , that is following

$$\operatorname{Re}[\chi(\omega)] = \int_{-\infty}^{\infty} \chi_{\text{even}}(t) \cos \omega t dt \quad \chi_{\text{even}}(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \operatorname{Re}[\chi(\omega)] \cos \omega t d\omega$$

The odd component of the impulse response function  $\chi_{\text{odd}}(t)$  is related to the even component by  $\chi_{\text{odd}}(t) = (\operatorname{sgn}(t))(\chi_{\text{even}}(t))$  that we re-write as follows

$$\chi_{\text{odd}}(t) = (\operatorname{sgn}(t))(\chi_{\text{even}}(t)) \quad \chi_{\text{even}}(t) = (\operatorname{sgn}(t))(\chi_{\text{odd}}(t))$$

This above relation is Kramer-Kronig's relation in time domain. Thus we see odd component is Hilbert Transform of even component and vice-versa.

The imaginary part of the susceptibility  $\operatorname{Im}[\chi(\omega)]$  can then be constructed since it is the Fourier ‘sine’ transform of the odd component.

$$\operatorname{Im}[\chi(\omega)] = -\int_{-\infty}^{\infty} \chi_{\text{odd}}(t) \sin \omega t dt \quad \chi_{\text{odd}}(t) = -\frac{1}{2\pi} \int_{-\infty}^{\infty} \operatorname{Im}[\chi(\omega)] \sin \omega t d\omega$$

Many observable quantities obey the Kramer-Kronig relations. For instance the electric susceptibility describes the electric polarization of a material responds to an applied electric field. This response must be causal so the real and imaginary parts of the electric susceptibility  $\chi_e(\omega)$  must be related by the Kramer-Kronig relations. This is also true for the electric modulus  $M(\omega)$ , magnetic susceptibility  $\chi_m(\omega)$ , the electrical conductivity, the thermal conductivity, and the dielectric constant  $\varepsilon(\omega)$ , stress compliance  $J(\omega)$  etc.

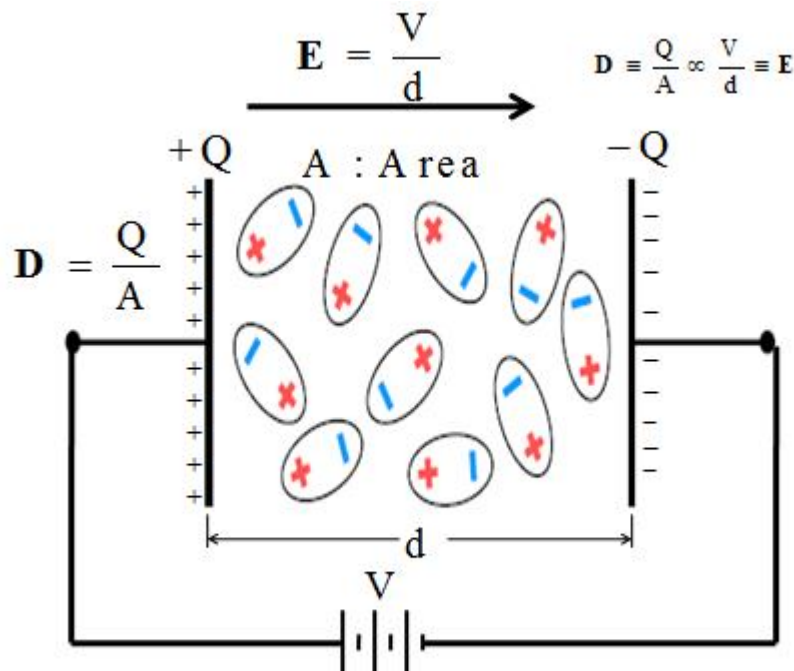


Sometimes it is experimentally easier to measure the real part (or the imaginary part) of the susceptibility- in frequency domain. The Kramer-Kronig relations then are utilized to calculate the part that is difficult to measure. If both real and imaginary parts can be measured, it is possible to check for experimental errors using the Kramer-Kronig relations. If susceptibility is calculated theoretically, it is a good idea to check and see if it satisfies the Kramer-Kronig relations. It should be considered a serious error to present a result that violates causality-and Kramer-Kronig relations.

### 19. Some Application to Electromagnetic Interactions

The concepts presented above are empirical descriptions of phenomena, that is the concept of a primary response function or susceptibility  $\chi(t)$ , is like a time dependent shear compliance  $J(t)$ , time dependent permittivity  $\epsilon(t)$ , time dependent magnetic permeability  $\mu(t)$  time dependent shear modulus  $G(t)$ , time dependent Electric Modulus  $M(t)$  or a time dependent magnetic susceptibility  $\chi_m(t)$  or time dependent electric-susceptibility  $\chi_e(t)$  etc. that do not involve understanding a given material, but are just general functions within which a discussion of the response to perturbation can be considered in a generic sense.

In our brief description about Electromagnetic waves travelling in the media we will discussed polarization concept. Again to begin with consider the mechanisms of relaxation we can first consider an extremely simple system, a system of molecular-sized dipoles subjected to an electric field. Interactions between the dipoles, lead to a retardation of rotation. This partial barrier to rotation leads to a finite time of relaxation to the oriented state.



**Figure-4: Random orientation of dipoles that take part in Polarization Process**

Consider an idealized dipole in a liquid state such as water molecules, Figure-4. The natural polarity of the water molecules is randomly oriented due to ‘thermal motion’ of the molecules. There is no bulk polarization of the water. When an electric field,  $\mathbf{E}$  is applied to the water a preferred direction of orientation of the water-molecule dipoles ‘develops in time’. The bulk sample is polarized to an orientation polarization of  $\mathbf{P}$ . This orientation represents a balance between 1) the applied electric field times the susceptibility of the molecules to orientation times the number of molecules per volume; and 2) the randomization of dipole orientation caused by thermal motion,  $3kT$ . The motion of water molecules is considered to be entirely rotational in this case. This value of  $\mathbf{P}$  is reached after some duration of time and is the predicted equilibrium value (or a steady state value), and we will use relation  $\mathbf{P} = \epsilon_0 \chi_e \mathbf{E}$ . This we will use to study the Kramer Kronig relation to get the formulas for  $\epsilon_r$ .

Because there is one simple process involved in the ‘relaxation’ of water molecules from the ‘strained’ state to the ‘equilibrium’ state the relaxation of a simple dipole displays a ‘single relaxation mode’. The constraints on relaxation, here interaction between dipoles, slows down the relaxation process (i.e. damping) and lead to a characteristic time ( $\tau$ ) associated with the relaxation towards equilibrium. Relaxation of this type is usually associated with an exponential decay function ( $\sim e^{-t/\tau}$ ) i.e. the function never reaches equilibrium in a finite time. For this reason, the relaxation time i.e.  $\tau$  is taken as the point when  $\frac{100}{e}$  % or 37% of the molecules have reached the equilibrium state. The time  $\tau$  is a natural factor to normalize time for such a process, i.e.  $t/\tau$  is a natural unit to measure time for a given simple relaxation process. We describe this simple relaxation (or retardation) process by following dynamic equation

$$\tau \epsilon \frac{d\mathbf{E}(t)}{dt} + \epsilon \mathbf{E}(t) = \mathbf{D}(t)$$

Where  $\mathbf{E}$  is Electric Field, which is Potential per unit distance  $\mathbf{E} = V/d$ ,  $\mathbf{D}$  is Dielectric Displacement of charges described as  $\mathbf{D} = Q/A$ . Where  $Q$  is the charge, and  $A$  is electrode area, the  $V$  is the potential across the electrode plates separated by dielectric of distance  $d$  (Figure-4). We have for a dielectric system  $\mathbf{D} \equiv (Q/A) \propto (V/d) \equiv \mathbf{E}$  with  $\mathbf{D} = \epsilon \mathbf{E}$ . This Electric Field Relaxation Equation described above has a relaxing electric  $\mathbf{E}(t) = \frac{1}{\epsilon \tau} e^{-t/\tau}$ , for  $t \geq 0$  with ‘unit impulse’ forced Dielectric Displacement,  $\mathbf{D}(t) = \delta(t)$  as applied as forcing function at  $t = 0$ ; with condition  $\mathbf{E}(t) = 0$  for  $t < 0$ . This is called ‘single-relaxation mode’-a Debye relaxation: and is also Green’s function of the system. Thus our susceptibility or impulse response is  $\chi(t) = \frac{1}{\epsilon \tau} e^{-t/\tau}$ . Most relaxations in polymers are much more complex than that of a simple dipole responding to an electric field.

## 20. Applying Kramer-Kronigs relation to get dispersion formulas for dissipation and loss for dielectric

This we apply to a specific application of Electromagnetic waves travelling through medium. In vacuum the speed of electromagnetic wave is  $c$  where  $c = 1/\sqrt{\epsilon_0 \mu_0}$  with  $\epsilon_0$ ,  $\mu_0$  as permittivity and permeability of free space (vacuum). The speed of wave in medium is  $c/n$ , where  $n$  is the refractive index of medium. Thus, the speed of wave in media is  $c/n = 1/\sqrt{\epsilon_0 \mu_0 \epsilon_r \mu_r}$ . The refractive index can be expressed in term

of relative permeability  $\mu_r$  and relative permittivity  $\varepsilon_r$  as  $n = \sqrt{\varepsilon_r \mu_r}$ . If we consider majority cases we have  $\mu_r \approx 1$  thus  $n \approx \sqrt{\varepsilon_r}$ .

The reason that medium affects the wave propagation is that the Electric Field  $\mathbf{E}$  causes polarization  $\mathbf{P}$  of the material. The polarization is related to the Electric Field by the relation  $\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E}$ , where  $\chi_e$  is the ‘electric-susceptibility’. The electric displacement is the sum of that in vacuum i.e.  $\varepsilon_0 \mathbf{E}$  and due to polarization  $\mathbf{P}$ . That we write as

$$\mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} = \varepsilon_0 \mathbf{E} + \varepsilon_0 \chi_e \mathbf{E}$$

$$\mathbf{D} = \varepsilon_0 (1 + \chi_e) \mathbf{E}$$

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$$

In this above application the input force is  $\mathbf{E}$  and the material’s response is  $\mathbf{P}$ . Consequently the relevant response function is electric susceptibility  $\chi_e = \varepsilon_r - 1$ , which is the factor of proportionality between  $\mathbf{E}$  and  $\mathbf{P}$ , as we stated earlier as  $\mathbf{P} = \varepsilon_0 \chi_e \mathbf{E}$ . We stress here, that incorrect result would be obtained if we either have relative permittivity  $\varepsilon_r$  or refractive index  $n$  as response functions.

The complex relative permittivity is conventionally written as  $\varepsilon_r(\omega) = \text{Re}[\varepsilon_r(\omega)] + i \text{Im}[\varepsilon_r(\omega)]$ .

Inserting this into  $\chi_e(\omega) = \varepsilon_r(\omega) - 1 = (\text{Re}[\varepsilon_r(\omega)] - 1) + i(\text{Im}[\varepsilon_r(\omega)])$ , and using obtained Krammer-

Kronig Relation i.e.  $\text{Re}[\bar{\chi}(\omega)] = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}[\bar{\chi}(\omega')]}{\omega' - \omega} d\omega'$  and  $\text{Im}[\bar{\chi}(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega' - \omega} d\omega'$ , we write

$$\text{Re}[\varepsilon_r(\omega)] - 1 = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}[\varepsilon_r(\omega')]}{\omega' - \omega} d\omega' \quad \text{Re}[\varepsilon_r(\omega)] = 1 + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}[\varepsilon_r(\omega')]}{\omega' - \omega} d\omega'$$

$$\text{Im}[\varepsilon_r(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Re}[\varepsilon_r(\omega')] - 1}{\omega' - \omega} d\omega'$$

We have discussed earlier that response function  $\bar{\chi}(\omega) = \text{Re}[\bar{\chi}(\omega)] + i \text{Im}[\bar{\chi}(\omega)] = \int_0^{\infty} d\tau \chi(\tau) e^{i\omega\tau}$  as

defined, having real part as even and imaginary part as odd functions in  $\omega$ . As we saw

$\chi_e = \varepsilon_r - 1 = (\text{Re}[\varepsilon_r] - 1) + i(\text{Im}[\varepsilon_r])$ , implies that the real and imaginary parts of  $\varepsilon_r$  are respectively

even and odd functions of  $\omega$  too, i.e.  $\text{Re}[\varepsilon_r(\omega)] = \text{Re}[\varepsilon_r(-\omega)]$  and  $\text{Im}[\varepsilon_r(-\omega)] = -\text{Im}[\varepsilon_r(\omega)]$ . This

implies the dispersion relation  $\text{Re}[\varepsilon_r] = 1 + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}[\varepsilon_r(\omega')]}{\omega' - \omega} d\omega'$  and  $\text{Im}[\varepsilon_r(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Re}[\varepsilon_r(\omega')] - 1}{\omega' - \omega} d\omega'$  can

be written as integrals over positive frequencies only, i.e. using the modified formula

$\text{Re}[\bar{\chi}(\omega)] = \frac{2}{\pi} \int_0^{\infty} \frac{\omega' \text{Im}[\bar{\chi}(\omega')]}{\omega'^2 - \omega^2} d\omega'$  and  $\text{Im}[\bar{\chi}(\omega)] = -\frac{2\omega}{\pi} \int_0^{\infty} \frac{\text{Re}[\bar{\chi}(\omega')]}{\omega'^2 - \omega^2} d\omega'$  we get the following

$$\text{Re}[\varepsilon_r(\omega)] = 1 + \frac{2}{\pi} \int_0^{\infty} \frac{\omega' \text{Im}[\varepsilon_r(\omega')]}{\omega'^2 - \omega^2} d\omega' \quad \text{Im}[\varepsilon_r(\omega)] = -\frac{2\omega}{\pi} \int_0^{\infty} \frac{\text{Re}[\varepsilon_r(\omega')] - 1}{\omega'^2 - \omega^2} d\omega'$$

The above relations are of practical significance, since we can measure dispersion in loss or in dissipation for positive frequencies. In some literatures the  $\varepsilon_\infty$  is used like  $\varepsilon_\infty = 1$ , and following Kramer-Kronigs relation are used

$$\operatorname{Re}[\varepsilon_r(\omega)] = \varepsilon_\infty + \frac{2}{\pi} \int_0^\infty d\omega' \frac{\omega' \operatorname{Im}[\varepsilon_r(\omega')]}{\omega'^2 - \omega^2}; \quad \operatorname{Im}[\varepsilon_r(\omega)] = -\frac{2\omega}{\pi} \int_0^\infty d\omega' \frac{\operatorname{Re}[\varepsilon_r(\omega')] - \varepsilon_\infty}{\omega'^2 - \omega^2}$$

Physically  $\varepsilon_\infty$  implies the value at frequency  $\omega = \infty$  or in time domain this is initial value of un-relaxed state, that is  $\varepsilon(t) = \varepsilon_U = \varepsilon_\infty$  at  $t = 0$ .

## 21. Using the dispersion relations of dielectric for obtaining complex refractive index

The physical meaning above dispersion relation is used when the complex refractive index gets formed by above relations i.e.  $n(\omega) \equiv \operatorname{Re}[n(\omega)] + i \operatorname{Im}[n(\omega)]$ . The wave vector, or propagation constant of Electromagnetic Wave  $k = \omega/c$  in vacuum becomes  $k = n\omega/c$  in medium. Hence a propagating Electromagnetic Wave becomes as follows

$$\begin{aligned} \exp(i(kx - \omega t)) &= \exp\left(i\omega\left(\frac{n(\omega)}{c}x - t\right)\right) \\ &= \exp\left(-\frac{\operatorname{Im}[n(\omega)]}{c}\omega x\right) \exp\left(i\omega\left(\frac{\operatorname{Re}[n(\omega)]}{c}x - t\right)\right) \end{aligned}$$

The wave in a medium having refractive index as positive imaginary part therefore decays exponentially with distance. The amplitude decays by a factor  $e$  for every distance  $c/(\omega \operatorname{Im}[n])$  travelled; this is 'penetration depth'. But since  $n^2 = \varepsilon_r$  we have

$$\operatorname{Re}[\varepsilon_r(\omega)] = (\operatorname{Re}[n(\omega)])^2 - (\operatorname{Im}[n(\omega)])^2 \quad \operatorname{Im}[\varepsilon_r(\omega)] = 2(\operatorname{Re}[n(\omega)])(\operatorname{Im}[n(\omega)])$$

Consequently the relations  $\operatorname{Re}[\varepsilon_r(\omega)] = 1 + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Im}[\varepsilon_r(\omega')]}{\omega' - \omega} d\omega'$  and  $\operatorname{Im}[\varepsilon_r(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Re}[\varepsilon_r(\omega')] - 1}{\omega' - \omega} d\omega'$  can be regarded as constraints between the real refractive index and its imaginary part which measures absorptive properties. This is very remarkable that these two properties of medium should be related since a priori they would appear to be separate quantities! This connection between real and imaginary parts however follows from causality principle, and hence fundamental in nature. It is the frequency dependence of  $\operatorname{Re}[n(\omega)]$  for a transparent medium which causes it to separate the colors from initially white beam of light! The frequency dependence of  $\operatorname{Re}[n(\omega)]$  is termed as 'dispersion' and this phenomena is due to equations  $\operatorname{Re}[\varepsilon_r(\omega)] = 1 + \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Im}[\varepsilon_r(\omega')]}{\omega' - \omega} d\omega'$  and  $\operatorname{Im}[\varepsilon_r(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\operatorname{Re}[\varepsilon_r(\omega')] - 1}{\omega' - \omega} d\omega'$  called 'dispersion equations'. The above relations implies in physical sense that they provide a means of determining the frequency dependence of the real refractive index by measuring only the absorptions over all the frequencies.

## 22. ‘Single Time Relaxation’-in Stress-Strain Studies-the Debye Relaxation

Consider a creep experiment for a material that displays a single mode of relaxation. A shear stress (constant)  $\sigma_0$  is applied at time  $t = 0$  and the strain  $\gamma(t)$  develops with time. We can consider that the application of stress creates a new equilibrium state (steady-state, at time say  $t \uparrow \infty$ ) for the material that is related to the magnitude of stress that is applied,  $(\Delta J)\sigma_0$  where  $\Delta J$  is called the ‘relaxation strength’. The change in strain,  $d\gamma(t)/dt$  changes with time and reaches 0 when the system is at equilibrium (steady-state), i.e. where  $\gamma(t)|_{t \uparrow \infty} = \Delta J\sigma_0$  (a constant). For a ‘linear decay’, the rate of change of strain is proportional to the distance from the equilibrium value of strain-that is

$$\frac{d\gamma(t)}{dt} = K(\gamma(t) - \Delta J\sigma_0)$$

The solution to above, with initial condition  $\gamma(0) = 0$  is  $\gamma(t) = \Delta J\sigma_0(1 - e^{Kt})$  for  $t \geq 0$  with  $\gamma(t) = 0$  for  $t < 0$ ; by using Laplace Transform technique. We have used  $\mathcal{L}\{\Delta J\sigma_0 K\} = \frac{\Delta J\sigma_0 K}{s}$  and  $\mathcal{L}\left\{\frac{d\gamma(t)}{dt}\right\} = s\gamma(s) - \gamma(0)$ , where  $\mathcal{L}\{\gamma(t)\} = \gamma(s)$ , and  $\mathcal{L}^{-1}\left\{\frac{1}{s-K}\right\} = e^{Kt}$ .

With  $t = \tau$ , we have  $\frac{100}{e}$  % relaxed, means  $\gamma(t)|_{t=\tau} = 100\left(1 - \frac{1}{e}\right)$  % of final value i.e.  $\gamma(t)|_{t \uparrow \infty} = \Delta J\sigma_0$ , is reached. Putting in  $\gamma(t) = \Delta J\sigma_0(1 - e^{Kt})$ ,  $t = \tau$  and  $\gamma(t)|_{t=\tau} = \Delta J\sigma_0(1 - e^{-1})$ ; we get  $K = -1/\tau$ . For this case therefore the solution is given by

$$\gamma(t) = \Delta J\sigma_0(1 - e^{(-t/\tau)})$$

The relaxation time  $\tau$  reflects the order of the time required for the relaxation to occur. The relaxation strength  $\Delta J$  is usually difficult to describe as it reflects the response of the system as a whole, i.e. ‘for polarization of a simple molecular dipole, the dipole strength and the coupling of all dipoles in the system that leads to the response’.

From the above we infer  $\gamma(t) = \Delta J\sigma_0(1 - e^{(-t/\tau)})$  is strain relaxation function, when the system is stressed by a constant step input stress,  $\sigma(t) = \sigma_0$  for  $t \geq 0$ . This is not the impulse response of the system, given by

$$\frac{\tau}{\Delta J} \frac{d\gamma(t)}{dt} + \frac{1}{\Delta J} \gamma(t) = \sigma(t)$$

For impulse response we need to apply unit impulse stress to above, i.e.  $\sigma(t) = \delta(t)$  at  $t = 0$ . Knowing the Laplace transform identity  $\mathcal{L}\{\delta(t)\} = 1$ , we use the Laplace transformation technique as done earlier to get  $\gamma(t) = (\Delta J/\tau)e^{-t/\tau}$ . So impulse response function (Green’s function) is  $(\Delta J/\tau)e^{-t/\tau}$  for  $t \geq 0$ . We used  $\mathcal{L}\{e^{-t/\tau}\} = \frac{\tau}{\tau s + 1}$ .

### 23. Obtaining dynamic compliance $\bar{J}(\omega)$ from harmonic forcing function

Consider the application of the simple relaxation model given above to a dynamic mechanical measurement of the dynamic compliance  $\bar{J}(\omega)$ ; is a complex quantity like  $\bar{\chi}(\omega)$  discussed earlier. For this case the equilibrium (steady-state) value,  $\Delta J \sigma_0$  is not constant but is  $\Delta J \sigma(t)$ , since  $\sigma(t) = \sigma_0 e^{-i\omega t}$  i.e. harmonic stress. Then we have,

$$\begin{aligned}\frac{d\gamma(t)}{dt} &= \left(-\frac{1}{\tau}\right)(\gamma(t) - \Delta J \sigma(t)), \quad \sigma(t) = \sigma_0 e^{-i\omega t} \\ \frac{d\gamma(t)}{dt} &= \left(-\frac{1}{\tau}\right)(\gamma(t) - \Delta J \sigma_0 e^{-i\omega t})\end{aligned}$$

From the previous discussion of response function  $x(t) = (\bar{\chi}(\omega))(F_0 e^{-i\omega t})$  we know that the resulting strain can be expressed as,

$$\gamma(t) = (\bar{J}(\omega))(\sigma_0 e^{-i\omega t})$$

By substitution of this expression into the differential equation and solving for the dynamic compliance,  $\bar{J}(\omega)$ , we write the following

$$\begin{aligned}\frac{d\gamma(t)}{dt} &= \left(-\frac{1}{\tau}\right)(\gamma(t) - \Delta J \sigma_0 e^{-i\omega t}) \\ (\bar{J}(\omega))(-i\omega \sigma_0 e^{-i\omega t}) &= \left(-\frac{1}{\tau}\right)((\bar{J}(\omega))(\sigma_0 e^{-i\omega t}) - \Delta J \sigma_0 e^{-i\omega t}) \\ \bar{J}(\omega) &= \frac{\Delta J}{1 - i\omega\tau} = \frac{\Delta J}{1 + \omega^2\tau^2} + i \frac{\Delta J \omega\tau}{1 + \omega^2\tau^2}\end{aligned}$$

Does Fourier Transformation of Green's Function has connection to Dynamic Compliance? We have Green's Function for the equation

$$\tau \frac{d\gamma(t)}{dt} + \gamma(t) = \Delta J \sigma(t); \quad \sigma(t) = \delta(t)$$

$$\gamma_{green}(t) = (\Delta J / \tau) e^{-t/\tau}; \quad t \geq 0$$

Using  $\mathcal{F}\{e^{-t/\tau} u(t)\} = \frac{\tau}{1+i\omega\tau}$  we write the following

$$J(\omega) = \mathcal{F}\left\{(\Delta J / \tau) e^{-t/\tau}\right\} = \frac{\Delta J}{1 + i\omega\tau} = \frac{\Delta J}{1 + \omega^2\tau^2} - i \frac{\Delta J \omega\tau}{1 + \omega^2\tau^2}$$

We compare with the obtained relation  $\bar{J}(\omega) = \frac{\Delta J}{1-i\omega\tau}$  and find similarity with Fourier Transform of the Green's function of the dynamic equation of system, i.e.  $J(\omega) = \frac{\Delta J}{1+i\omega\tau}$ . Nevertheless we note in our derivation of  $\bar{J}(\omega)$  we have used harmonic excitation of the form  $\sigma(t) = \sigma_0 e^{-i\omega t}$ . We could also use the excitation as  $\sigma(t) = \sigma_0 e^{i\omega t}$ , in that case repeating the above steps, we would get  $J(\omega) = \frac{\Delta J}{1+i\omega\tau}$  as shown below

$$\begin{aligned}\frac{d\gamma(t)}{dt} &= \left(-\frac{1}{\tau}\right)\left(\gamma(t) - \Delta J \sigma_0 e^{i\omega t}\right) \\ (J(\omega))(i\omega\sigma_0 e^{i\omega t}) &= \left(-\frac{1}{\tau}\right)\left((J(\omega))(\sigma_0 e^{i\omega t}) - \Delta J \sigma_0 e^{i\omega t}\right) \\ J(\omega) &= \frac{\Delta J}{1+i\omega\tau}\end{aligned}$$

The above expression is also dynamic compliance  $J(\omega)$ , which is complex conjugate of  $\bar{J}(\omega)$  and be used too. Here we mention that dynamic compliance is indeed Fourier transform of the Green's function of the system.

#### 24. Some interesting observations about dynamic compliance $\bar{J}(\omega)$

This expression for the dynamic compliance from a simple relaxation is called a "Debye-process". The real and imaginary parts of this complex compliance can be obtained as,

$$\begin{aligned}\bar{J}(\omega) &= \frac{\Delta J}{1-i\omega\tau} \\ \bar{J}(\omega) &\equiv \text{Re}[\bar{J}(\omega)] + i \text{Im}[\bar{J}(\omega)] = \frac{\Delta J}{1+\omega^2\tau^2} + i \frac{\omega\tau\Delta J}{1+\omega^2\tau^2}\end{aligned}$$

From above we see  $\text{Re}[\bar{J}(-\omega)] = \text{Re}[\bar{J}(\omega)]$  is even function and  $\text{Im}[\bar{J}(-\omega)] = -\text{Im}[\bar{J}(\omega)]$  is odd function.

The Real part can be written as

$$\begin{aligned}\text{Re}[\bar{J}(\omega)] &= \frac{\Delta J}{1+\omega^2\tau^2} = \frac{1}{\omega\tau} \left( \frac{\Delta J}{\frac{1}{\omega\tau} + \omega\tau} \right) \\ &= 10^{-\log \omega\tau} \frac{\Delta J}{10^{-\log \omega\tau} + 10^{\log \omega\tau}}\end{aligned}$$

We see  $\lim_{\omega \downarrow 0} \text{Re}[\bar{J}(\omega)] = \lim_{\omega \downarrow 0} \left( \frac{\Delta J}{1+\omega^2\tau^2} \right) = \Delta J$  and  $\lim_{\omega \uparrow \infty} \text{Re}[\bar{J}(\omega)] = \lim_{\omega \uparrow \infty} \left( \frac{\Delta J}{1+\omega^2\tau^2} \right) = 0$ . Placing  $\omega\tau = x$  we have  $\text{Re}[\bar{J}(\omega)] = \frac{\Delta J}{1+x^2}$ . The derivative is

$$\begin{aligned}\frac{d}{dx} \operatorname{Re}[\bar{J}(\omega)] &= -2\Delta J x(1+x^2)^{-1} \\ \frac{d}{d(\omega\tau)} \operatorname{Re}[\bar{J}(\omega)] &= -2\Delta J \frac{\omega\tau}{1+\omega^2\tau^2} = -2 \operatorname{Im}[\bar{J}(\omega)] \\ \operatorname{Im}[\bar{J}(\omega)] &= -\frac{1}{2} \frac{d}{d(\omega\tau)} \operatorname{Re}[\bar{J}(\omega)]\end{aligned}$$

and this is maximum at  $x = \omega\tau = 1$ , with maximum value of rate of change of  $\operatorname{Re}[\bar{J}(\omega)]$  as  $-\Delta J$ . From above observations we can integrate the last expression and write

$$\operatorname{Re}[\bar{J}(\omega)] = -2 \int \operatorname{Im}[\bar{J}(\omega)] d(\omega\tau) + C$$

Where  $C$  is initial value of  $\operatorname{Re}[\bar{J}(\omega)]$  which in this case is  $\Delta J$ , i.e. value at  $\operatorname{Re}[\bar{J}(\omega)]_{\omega=0} = \Delta J$ . This is because  $\left(\int f^{(1)}\right) = f - f(0)$ . So we have

$$\begin{aligned}\operatorname{Re}[\bar{J}(\omega)] &= -2 \int \operatorname{Im}[\bar{J}(\omega)] d(\omega\tau) + \Delta J \\ \operatorname{Im}[\bar{J}(\omega)] &= -\frac{1}{2} \frac{d}{d(\omega\tau)} \operatorname{Re}[\bar{J}(\omega)]\end{aligned}$$

Here we see derivative of storage compliance i.e.  $\operatorname{Re}[\bar{J}(\omega)]$  is proportional to loss compliance i.e.  $\operatorname{Im}[\bar{J}(\omega)]$ , or other way we can say integral of loss compliance, i.e.  $\operatorname{Im}[\bar{J}(\omega)]$  is proportional to storage compliance i.e.  $\operatorname{Re}[\bar{J}(\omega)]$ . This is similar (but not the same) to Kramer-Kronigs relationship relating real and imaginary parts of Causal system discussed earlier i.e.

$$\operatorname{Re}[\bar{J}(\omega)] = \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\operatorname{Im}[\bar{J}(\omega')]}{\omega' - \omega} \quad \operatorname{Im}[\bar{J}(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\operatorname{Re}[\bar{J}(\omega')]}{\omega' - \omega}$$

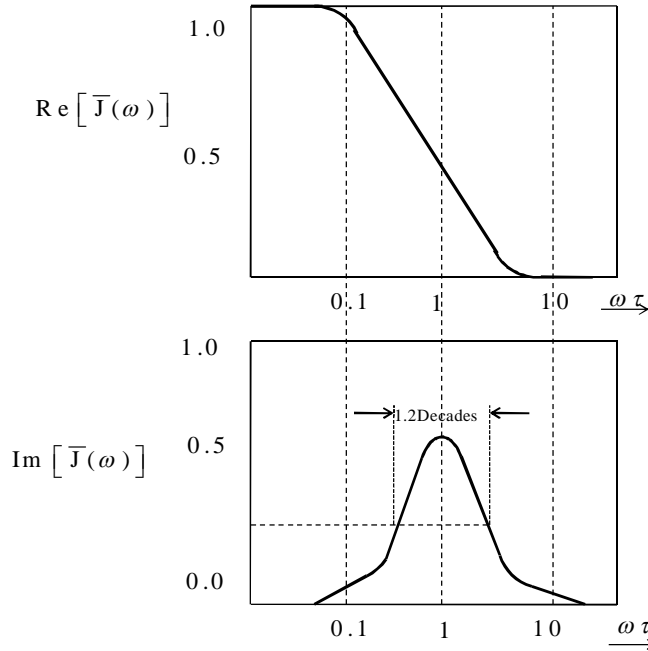
Thus  $\operatorname{Re}[\bar{J}(\omega)]$  is monotonically falling curve from  $\Delta J$  at very-very low  $\omega$ ; then falling off at maximum rate at  $\omega = (1/\tau)$  with rate as  $-\Delta J$  when  $\operatorname{Re}[\bar{J}(\omega)] = \frac{\Delta J}{2}$  and ultimately rolling off to 0 at very-very high frequency. The real part of the dynamic compliance shows a steep decay at  $\omega\tau = 1$ . When the system is excited or probed with times longer than the relaxation time (lower frequency) relaxation is complete and a high compliance (full compliance) is observed, that is  $\Delta J$ . At high frequency (short times) the system cannot display relaxation so the compliance goes to 0.

The imaginary part can be written



$$\begin{aligned} \text{Im}[\bar{J}(\omega)] &= \frac{\Delta J \omega \tau}{1 + \omega^2 \tau^2} = \frac{\Delta J}{\frac{1}{\omega \tau} + \omega \tau} \\ &= \frac{\Delta J}{10^{-\log \omega \tau} + 10^{\log \omega \tau}} \end{aligned}$$

We see  $\lim_{\omega \downarrow 0} \text{Im}[\bar{J}(\omega)] = \lim_{\omega \downarrow 0} \left( \frac{\Delta J \omega \tau}{1 + \omega^2 \tau^2} \right) = 0$  and  $\lim_{\omega \uparrow \infty} \text{Im}[\bar{J}(\omega)] = \lim_{\omega \uparrow \infty} \left( \frac{\Delta J \omega \tau}{1 + \omega^2 \tau^2} \right) = 0$ . With  $x = \omega \tau$  we write  $\text{Im}[\bar{J}(\omega)] = \Delta J \left( \frac{x}{1+x^2} \right)$  and differentiating  $\left( \frac{d(\text{Im}[\bar{J}(\omega)])}{dx} \right) = 0$  yields  $x = 1$ . So we say at  $x = \omega \tau = 1$  gives maximum value with  $\max(\text{Im}[\bar{J}(\omega)])_{\omega \tau = 1} = \frac{\Delta J}{2}$ . So the function  $\text{Im}[\bar{J}(\omega)]$  should be symmetric (about  $\omega \tau = 1$ ) on a linear-log plot of loss compliance versus frequency. We note that  $\omega \tau = 1$  is the point when  $\text{Re}[\bar{J}(\omega)] = \Delta J / 2$  where maximum rate of change of  $\text{Re}[\bar{J}(\omega)]$  occurs, and also at this point  $\omega \tau = 1$  gives peak value of loss compliance  $\text{Im}[\bar{J}(\omega)]$  with value  $\Delta J / 2$ .



**Figure-5: Schematic plots of dissipative systems showing real part and imaginary part of dynamic compliance vis-à-vis frequency associated with Debye process (with  $\Delta J = 1$ )**

## 25. Relationship between the Loss and Storage Compliance for a Debye-Process

The dynamic compliance  $\bar{J}(\omega)$  has real and imaginary parts; as observed. The real part we say as storage compliance and the imaginary part we say as loss compliance. The maximum in the loss curve i.e.

$\text{Im}[\bar{J}(\omega)]$  and the steepest decay (i.e. rate of change in  $\text{Re}[\bar{J}(\omega)]$  in the storage compliance curve i.e.  $\text{Re}[\bar{J}(\omega)]$  both occur at  $\omega\tau = 1$  (Figure-5) indicating a relationship between the two processes. This indicates that the derivative of the storage curve  $\text{Re}[\bar{J}(\omega)]$  may have some relationship to the loss curve  $\text{Im}[\bar{J}(\omega)]$  or the integral of the loss curve  $\text{Im}[\bar{J}(\omega)]$  is related to the storage curve  $\text{Re}[\bar{J}(\omega)]$  -this we have demonstrated earlier. Integration of the equation  $\text{Im}[\bar{J}(\omega)]$  above for the loss compliance yields the following

$$\begin{aligned} & \int_{-\infty}^{+\infty} (\text{Im}[\bar{J}(\omega\tau)]) d(\log \omega\tau) \\ &= \int_{-\infty}^{\infty} \left( \frac{\Delta J}{10^{-\log \omega\tau} + 10^{\log \omega\tau}} \right) d(\log \omega\tau) = \frac{\pi}{2 \ln 10} \Delta J \end{aligned}$$

The above integral we calculate by taking  $I = \int_{-\infty}^{\infty} \frac{dx}{10^{-x} + 10^x}$ , with  $x = \log \omega\tau$  and  $\Delta J = 1$

$$\begin{aligned} I &= \int_{-\infty}^{\infty} \frac{dx}{10^{-x} + 10^x} = \int_{-\infty}^{\infty} \frac{10^x dx}{1 + 10^{2x}} \\ 10^x &= y, \quad x \ln 10 = \ln y; \quad \ln 10 = \frac{1}{y} \frac{dy}{dx} \\ y dx &= \frac{dy}{\ln 10}; \quad 10^x dx = \frac{dy}{\ln 10} \end{aligned}$$

The limits in  $y$  are now  $10^{-\infty} = 0$  to  $10^{\infty} = \infty$  and we have

$$\begin{aligned} I &= \int_{-\infty}^{\infty} \frac{10^x dx}{1 + 10^{2x}} = \int_0^{\infty} \frac{y dx}{1 + y^2} \\ &= \int_0^{\infty} \frac{dy}{\ln 10 (1 + y^2)} = \frac{1}{\ln 10} \int_0^{\infty} \frac{dy}{y^2 + 1} \\ &= \frac{1}{\ln 10} [\tan^{-1} y]_{y=0}^{y=\infty} \\ &= \frac{1}{\ln 10} \left( \frac{\pi}{2} \right) \end{aligned}$$

So the integral of the loss curve is proportional to the strength of the relaxation  $\int_{-\infty}^{+\infty} (\text{Im}[\bar{J}(\omega\tau)]) d(\log \omega\tau) = \left( \frac{\pi}{2 \ln 10} \right) \Delta J$ . This is similar (but not the same) to a direct result of the Kramer-Kronig relationship discussed earlier that is  $\text{Re}[\bar{J}(\omega)] = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Im}[\bar{J}(\omega')]}{\omega' - \omega} d\omega'$  and

$\text{Im}[\bar{J}(\omega)] = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\text{Re}[\bar{J}(\omega')]}{\omega' - \omega} d\omega'$ . Therefore it is impossible to have loss compliance  $\text{Im}[\bar{J}(\omega)]$  without a corresponding change in the storage compliance  $\text{Re}[\bar{J}(\omega)]$  (in frequency domain).

## 26. Identifying Oscillation or Relaxation from Debye to non-Debye

The total width at half-height for the Debye-process relaxation's loss compliance curve  $\text{Im}[\bar{J}(\omega)]$  in the Figure-5 above is 1.2 decades. This is the lower limit for a relaxation process, that is, more complicated (non-Debye relaxations) relaxations display a broader loss compliance  $\text{Im}[\bar{J}(\omega)]$  peak. The loss curve  $\text{Im}[\bar{J}(\omega)]$  for a simple harmonic oscillator is single valued and a damped harmonic oscillator displays a peak with a half-width much narrower than that of the Debye-process of relaxation (1.2 decades). Then the width of the loss compliance curve can be used to distinguish between a relaxation process and an oscillatory process (Figure-6). A fundamental difference between an oscillating system and a relaxing system is that an oscillating system displays a moment of inertia, i.e. it stores energy, while a relaxing system only dissipates energy.

In the examples so far for relaxation dynamics we have seen first order differential equations (describing dissipative systems), and we described from them the concept of susceptibility  $\bar{\chi}(\omega)$ , or  $\bar{J}(\omega)$  in the stress-strain relaxation model, electric field relaxation model, velocity relaxation models in earlier sections. The relaxation system can be second order or even fractional order differential equation. The oscillatory relaxation with damping is given by following second order differential equation

$$m \frac{d^2 x(t)}{dt^2} + \frac{m}{\tau} \frac{dx(t)}{dt} + m\omega_0^2 x(t) = f(t)$$

where  $x \equiv x(t)$  position variable in time. This is a damped oscillator system where Forcing function is  $f(t)$ . Exciting this system with a harmonic force of a single frequency  $\omega$  i.e.  $f(t) = F_0 e^{-i\omega t}$ , we will get  $x(t) = \bar{\chi}(\omega) F_0 e^{-i\omega t}$ . Where

$$\begin{aligned} \bar{\chi}(\omega) &= -\frac{1}{m} \left( \frac{1}{\omega^2 + i\omega/\tau - \omega_0^2} \right) = \frac{(1/m)}{\omega_0^2 - \omega^2 - i\omega/\tau} \\ &= \frac{-(1/m)(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2) + (\omega^2/\tau^2)} + i \frac{(1/m)(\omega/\tau)}{(\omega^2 - \omega_0^2) + (\omega^2/\tau^2)} \\ &= \frac{(-1/m)}{(\omega - \omega_1)(\omega - \omega_2)} \\ \chi(\omega) &= [\bar{\chi}(\omega)]_{\omega \rightarrow -\omega} = \frac{(1/m)}{\omega_0^2 - \omega^2 + i\omega/\tau} \end{aligned}$$

We have  $\omega_{1,2} = (-i/2\tau) \pm \tilde{\omega}$  with  $\tilde{\omega} = \sqrt{\omega_0^2 - (1/4\tau^2)}$ , roots of  $(\omega_0^2 - \omega^2 - i\omega/\tau) = 0$ . Here the response function  $\bar{\chi}(\omega)$  has two simple poles at  $\omega_1 = \tilde{\omega} - i(\frac{1}{2\tau})$  and at  $\omega_2 = -\tilde{\omega} - i(\frac{1}{2\tau})$ .

Fourier inverse of  $\chi(\omega) = [\bar{\chi}(\omega)]_{\omega \rightarrow -\omega}$  gives  $x(t) = (\frac{1}{m\tilde{\omega}} e^{-t/2\tau} \sin \tilde{\omega}t)u(t)$ ; where  $u(t)$  is unit step function. This response is response to force  $f(t) = \delta(t)$  unit impulse at  $t=0$  gives Green's function  $x_{green}(t) = (\frac{1}{m\tilde{\omega}} e^{-t/2\tau} \sin \tilde{\omega}t)$  for  $t \geq 0$ . This comes from following known Fourier transform pair

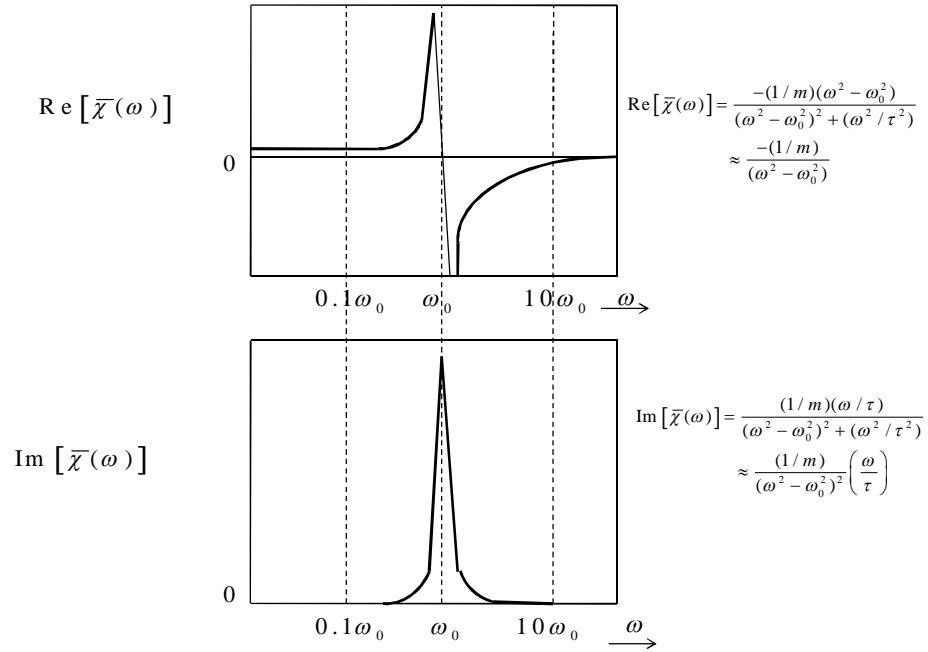
$$\mathcal{F} \{u(t)e^{-at} \sin b_0t\} = \frac{b_0}{b_0^2 + (a + i\omega)^2}$$

The roots of  $b_0^2 + (a + i\omega)^2 = 0$  are  $\omega_{1,2} = \pm b_0 + ia$  pair of simple poles for the function  $\frac{b_0}{b_0^2 + (a + i\omega)^2}$ . Comparing the poles of  $\chi(\omega) = \frac{1}{m} \left( \frac{1}{\omega_0^2 - \omega^2 + i\omega/\tau} \right)$ ; which is  $\omega_{1,2} = \pm \sqrt{\omega_0^2 - \frac{1}{4\tau^2}} + i(\frac{1}{2\tau}) = \pm \tilde{\omega} + i(\frac{1}{2\tau})$ ; we write  $b_0 \equiv \tilde{\omega} = \sqrt{\omega_0^2 - \frac{1}{4\tau^2}}$  and  $a \equiv \frac{1}{2\tau}$ , and thus the result  $x(t) = (\frac{1}{m\tilde{\omega}} e^{-t/2\tau} \sin \tilde{\omega}t)u(t)$ .

We have

$$\text{Re}[\bar{\chi}(\omega)] = \frac{-(1/m)(\omega^2 - \omega_0^2)}{(\omega^2 - \omega_0^2)^2 + (\omega^2/\tau^2)} \quad \text{Im}[\bar{\chi}(\omega)] = \frac{(1/m)(\omega/\tau)}{(\omega^2 - \omega_0^2)^2 + (\omega^2/\tau^2)}$$

For a very small damping we take the term  $(m/\tau) \approx 0$ , which gives  $\text{Re}[\bar{\chi}(\omega)] \approx \frac{-(1/m)}{(\omega^2 - \omega_0^2)}$  and  $\text{Im}[\bar{\chi}(\omega)] \approx \frac{(1/m)}{(\omega^2 - \omega_0^2)^2} \left( \frac{\omega}{\tau} \right)$ , that is a pure oscillatory system. The Real and Imaginary parts will take the shape in Figure-6.



**Figure-6: Real and Imaginary Part of susceptibility for oscillatory system**

We compare the two Figures-5 and 6. We observe that real part of the susceptibility of we called dynamic compliance for a dissipative system is monotonically decaying function, without any peak, and the function at low frequency to high frequency goes from full compliance towards zero. Whereas for a oscillatory decay the real part of the susceptibility (or dynamic compliance) show a peak at resonance frequency, and have values positive and negative at respective sides of resonance frequency. The loss curve (Imaginary part) looks the same that is for both the systems, is like a bell type curves. But the oscillatory system has a very narrow width. In the oscillatory system, if the damping is reduced to very small, the curve becomes narrower and sharper and for zero damping the loss curve is a delta function at resonance frequency (a single valued). The Debye dissipating system has loss curve as critical width of 1.2 Decades as mentioned in Figure-5, a narrower loss curve is thus indicative of an oscillatory system, while broader peaks are indicative of complex non-Debye relaxation systems.

## 27. Retardation response-the shear compliance $J(t)$ and dynamic shear compliance $\bar{J}(\omega)$ in detail derivation

For a ‘single-time’ process the stress,  $\sigma(t)$  and strain,  $\gamma(t)$  are related by

$$\tau \frac{d\gamma(t)}{dt} + \gamma(t) = \tau J_U \frac{d\sigma(t)}{dt} + J_R \sigma(t)$$

We define time dependent shear compliance  $J(t)$  as

$$J(t) = \frac{\gamma(t)}{\sigma(t)}$$

where  $\tau$  is the relaxation time (modulus base). The time dependent  $J(t)$  is real function. The subscript U is un-relaxed and subscript R denotes relaxed state. This implies  $J_U = J(t)|_{t=0}$  and  $J_R = J(t)|_{t \rightarrow \infty}$  are initial and steady state values of  $J(t)$  respectively. This equation is obtained by the use of a single exponential decay in the Boltzmann superposition equation. For Creep, put  $\sigma(t) = \sigma_0 u(t)$  a constant step load of stress ( $u(t)$  is unit step function) and the above equation becomes

$$\begin{aligned} \tau \frac{d\gamma(t)}{dt} + \gamma(t) &= \tau J_U \frac{d\sigma(t)}{dt} + J_R \sigma(t) & \sigma(t) &= \sigma_0 u(t), & \frac{du(t)}{dt} &= \delta(t) \\ \tau \frac{d\gamma(t)}{dt} + \gamma(t) &= \tau J_U \sigma_0 \delta(t) + J_R \sigma_0 u(t) \\ \tau \frac{d\left(\frac{\gamma(t)}{\sigma_0}\right)}{dt} + \left(\frac{\gamma(t)}{\sigma_0}\right) &= \tau J_U \delta(t) + J_R u(t); & J(t) &= \frac{\gamma(t)}{\sigma_0}; & \gamma(t)|_{t=0} &= 0 \\ \tau \frac{dJ(t)}{dt} + J(t) &= \tau J_U \delta(t) + J_R u(t) \end{aligned}$$

Using Laplace transform we get the following solution

$$\begin{aligned} \tau \frac{dJ(t)}{dt} + J(t) &= \tau J_U \delta(t) + J_R u(t); & J(0) &= 0, & \mathcal{L}\{u(t)\} &= \frac{1}{s}, & \mathcal{L}\{\delta(t)\} &= 1 \\ \tau (sJ(s) - J(0)) + J(s) &= \tau J_U + J_R \left(\frac{1}{s}\right) \\ J(s) &= \frac{\tau J_U}{1 + s\tau} + \frac{J_R}{s(1 + s\tau)} \\ J(s) &= \frac{\tau J_U}{1 + s\tau} + \left(\frac{J_R}{s} - \frac{\tau J_R}{1 + s\tau}\right) \\ J(t) &= J_R + (J_U - J_R)e^{-t/\tau}; & J_R &= J_U + \Delta J \\ &= J_U + \Delta J - \Delta J e^{-t/\tau} \\ J(t) &= J_U + \Delta J (1 - e^{-t/\tau}); & \Delta J &= J_R - J_U \end{aligned}$$

The retardation response  $J(t)$  to unit step input stress is plotted in Figure-7. We note that the obtained  $J(t)$  is not the impulse response function or the Green's function. We need Green's function to get the dynamic shear compliance  $\bar{J}(\omega)$ . Impulse Response Function is with placing  $\sigma(t) = \sigma_0 \delta(t)$  as shown below

$$\begin{aligned}
\tau \frac{d\gamma(t)}{dt} + \gamma(t) &= \tau J_U \frac{d\sigma(t)}{dt} + J_R \sigma(t) & \sigma(t) &= \sigma_0 \delta(t); & \frac{d\sigma(t)}{dt} &= \delta^{(1)}(t) \\
\tau \frac{d\gamma(t)}{dt} + \gamma(t) &= \tau J_U \sigma_0 \delta^{(1)}(t) + J_R \sigma_0 \delta(t) \\
\tau \frac{d\left(\frac{\gamma(t)}{\sigma_0}\right)}{dt} + \left(\frac{\gamma(t)}{\sigma_0}\right) &= \tau J_U \delta^{(1)}(t) + J_R \delta(t); & J(t) &= \frac{\gamma(t)}{\sigma_0}; & \gamma(t)|_{t=0} &= 0 \\
\tau \frac{dJ(t)}{dt} + J(t) &= \tau J_U \delta^{(1)}(t) + J_R \delta(t) \\
\tau s J(s) + J(s) &= \tau J_U \mathcal{L}\{\delta^{(1)}(t)\} + J_R \mathcal{L}\{\delta(t)\} \\
&= \tau J_U (s \mathcal{L}\{\delta(t)\} - \delta(0^-)) + J_R \mathcal{L}\{\delta(t)\} & \mathcal{L}\{\delta(t)\} &= 1, & \delta(0^-) &= 0 \\
(1 + s\tau) J(s) &= \tau s J_U + J_R \\
J(s) &= \frac{J_R}{(1 + s\tau)} + \frac{s\tau J_U}{(1 + s\tau)}; & J_R &= J_U + \Delta J \\
&= \frac{J_U}{1 + s\tau} + \frac{\Delta J}{1 + s\tau} + \frac{s\tau J_U}{(1 + s\tau)} = J_U + \frac{\Delta J}{1 + s\tau}
\end{aligned}$$

The inverse Laplace transforms of  $J(s) = J_U + \left(\frac{\Delta J}{1+s\tau}\right)$  gives impulse response function or Green's function

$$\begin{aligned}
J_{green}(t) &= \mathcal{L}^{-1}\{J_U\} + \mathcal{L}^{-1}\left\{\frac{\Delta J}{1+s\tau}\right\} \\
&= J_U \delta(t) + \frac{\Delta J}{\tau} e^{-t/\tau} u(t)
\end{aligned}$$

We observe that above  $J_{green}(t)$  is derivative of  $J(t) = J_U + \Delta J(1 - e^{-t/\tau})$  that was Creep solution with step input of stress. The dynamic shear compliance we get by following Fourier Transform of the Green's function, by using  $\mathcal{F}\{\delta(t)\} = 1$  and  $\mathcal{F}\{u(t)e^{-t/\tau}\} = \frac{\tau}{1+i\omega\tau}$

$$\begin{aligned}
J(\omega) &= \mathcal{F}\{J_{green}(t)\} \\
&= \mathcal{F}\left\{J_U \delta(t) + \Delta J \left(\frac{1}{\tau}\right) e^{-t/\tau} u(t)\right\} \\
&= J_U + \frac{\Delta J}{1+i\omega\tau} \\
\bar{J}(\omega) &= J_U + \frac{\Delta J}{1-i\omega\tau}
\end{aligned}$$

The dynamic shear compliance of the Debye process is

$$\begin{aligned}
\bar{J}(\omega) &= J_U + \frac{\Delta J}{1 - i\omega\tau} \\
&= J_U + \frac{J_R - J_U}{1 + \omega^2\tau^2} (1 + i\omega\tau) \\
&= \frac{J_U + J_U\omega^2\tau^2 + J_R + i\omega\tau J_R - J_U - i\omega\tau J_U}{1 + \omega^2\tau^2} \\
&= \frac{J_U(1 + \omega^2\tau^2) + J_R - J_U}{1 + \omega^2\tau^2} + i \frac{\omega\tau(J_R - J_U)}{1 + \omega^2\tau^2} \\
&= J_U + \frac{J_R - J_U}{1 + \omega^2\tau^2} + i \frac{\omega\tau(J_R - J_U)}{1 + \omega^2\tau^2}
\end{aligned}$$

The real and imaginary parts are

$$\text{Re}[\bar{J}(\omega)] = J_U + \frac{J_R - J_U}{1 + \omega^2\tau^2} = J_U + \frac{\Delta J}{1 + \omega^2\tau^2}, \quad \text{Im}[\bar{J}(\omega)] = \frac{\omega\tau(J_R - J_U)}{1 + \omega^2\tau^2} = \frac{\omega\tau(\Delta J)}{1 + \omega^2\tau^2}$$

## 28. Relaxation response-the shear modulus $G(t)$ and dynamic shear modulus $\bar{G}(\omega)$ (Reciprocal of shear compliance $J(t)$ )-detailed derivation

As we have obtained dynamic-shear-compliance  $\bar{J}(\omega)$ , we will obtain dynamic shear modulus. By taking the inverse of this expression for shear-compliance,  $J(t)$  we get shear-modulus  $G(t) = (1/J(t))$  and substituting  $J_R = J_U + \Delta J$ ;  $\Delta J > 0$ ,  $\bar{\tau} = \tau(J_U/J_R) = \tau(G_R/G_U)$ ,  $G_U = (1/J_U)$ ,  $G_R = (1/J_R)$  and  $\Delta G = G_U - G_R > 0$ . We have  $J_R > J_U$  then  $\bar{\tau}$  is smaller than  $\tau$ . That is the characteristic time (time-constant) for the shear modulus  $G(t)$  from the Debye-process i.e.  $\bar{\tau}$  is smaller than the characteristic time  $\tau$  for the shear compliance  $J(t)$ ; (Refer Figure-7). Now we formulate shear-modulus  $G(t)$ s case as following, where we give step strain input  $\gamma(t) = \gamma_0 u(t)$ , where  $u(t)$  is the unit step function, with initial condition  $\sigma(0) = 0$ , and obtain  $G(t)$  (i.e. response  $\sigma(t)$  for  $\gamma_0 = 1$ )

$$\tau \frac{d\gamma(t)}{dt} + \gamma(t) = \tau J_U \frac{d\sigma(t)}{dt} + J_R \sigma(t), \quad \gamma(t) = \gamma_0 u(t), \quad G(t) = \frac{\sigma(t)}{\gamma(t)} = \frac{1}{J(t)}$$

$$\tau \gamma_0 \delta(t) + \gamma_0 u(t) = \frac{\tau}{G_U} \frac{d\sigma(t)}{dt} + \frac{1}{G_R} \sigma(t), \quad \frac{\tau}{G_U} \frac{d\left(\frac{\sigma(t)}{\gamma_0}\right)}{dt} + \frac{1}{G_R} \frac{\sigma(t)}{\gamma_0} = u(t) + \tau \delta(t); \quad G(t) = \frac{\sigma(t)}{\gamma_0}$$

$$\frac{\tau}{G_U} \frac{dG(t)}{dt} + \frac{1}{G_R} G(t) = u(t) + \tau \delta(t) \quad \bar{\tau} = \tau \frac{G_R}{G_U}$$

$$\bar{\tau} \frac{dG(t)}{dt} + G(t) = G_R u(t) + \bar{\tau} G_U \delta(t);$$



Note for shear compliance  $J(t)$  case we have the following

$$\begin{aligned}\tau \frac{dJ(t)}{dt} + J(t) &= \tau J_U \delta(t) + J_R u(t) \\ J(t) &= J_R + (J_U - J_R) e^{-t/\tau}; \quad J_R = J_U + \Delta J \\ &= J_U + \Delta J - \Delta J e^{-t/\tau} \\ J(t) &= J_U + \Delta J (1 - e^{-t/\tau}); \quad \Delta J = J_R - J_U\end{aligned}$$

We use similar method by using Laplace Transformation we get the following for

$$\begin{aligned}\bar{\tau} \frac{dG(t)}{dt} + G(t) &= \bar{\tau} G_U \delta(t) + G_R u(t) \\ \bar{\tau} (sG(s) - G(0)) + G(s) &= \bar{\tau} G_U + G_R \left( \frac{1}{s} \right); \quad G(0) = 0 \\ G(s) &= \frac{\bar{\tau} G_U}{1 + s\bar{\tau}} + \frac{G_R}{s(1 + s\bar{\tau})} \\ G(s) &= \frac{\bar{\tau} G_U}{1 + s\bar{\tau}} + \left( \frac{G_R}{s} - \frac{\bar{\tau} G_R}{1 + s\bar{\tau}} \right) \\ G(t) &= G_R + (G_U - G_R) e^{-t/\bar{\tau}}; \quad G_R = G_U - \Delta G \\ &= G_U - \Delta G + \Delta G e^{-t/\bar{\tau}} \\ G(t) &= G_U - \Delta G (1 - e^{-t/\bar{\tau}}); \quad \Delta G = G_U - G_R\end{aligned}$$

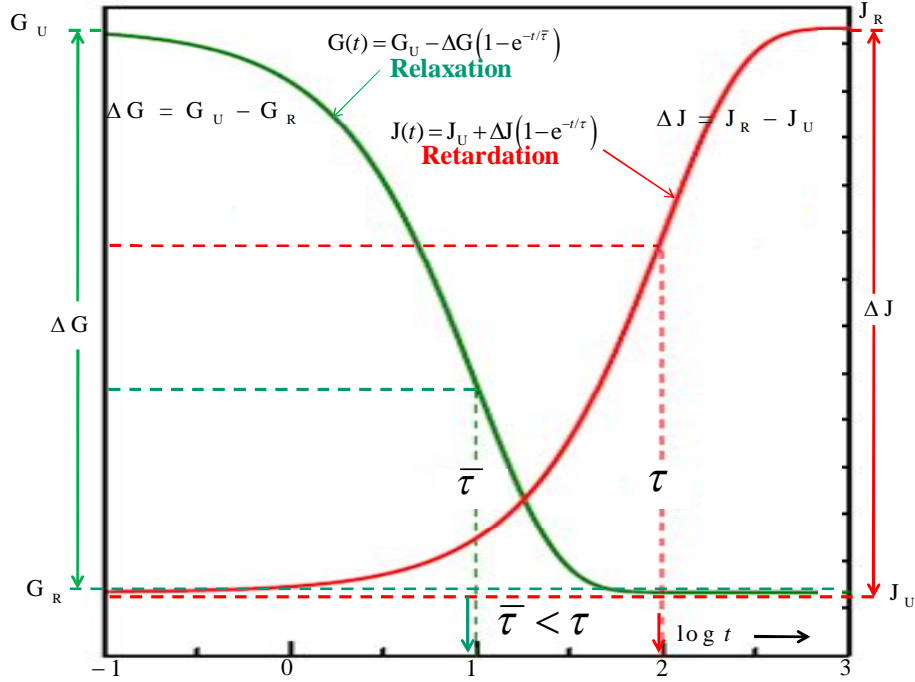
The responses  $G(t)$  and  $J(t)$  the response to unit-step of strain and unit-step of stress respectively are shown in Figure-7. The response  $G(t)$  is ‘relaxation’ while the response  $J(t)$  is termed as ‘retardation’. We note that  $G(t)$  obtained above is not Green’s function, as the excitation is step input  $\gamma(t) = \gamma_0 u(t)$ . We can repeat the steps as obtained for  $J_{green}(t)$ , but also we stated that the Green’s function is differentiation of the  $J(t)$ . Here we differentiate the obtained  $G(t) = G_U - \Delta G (1 - e^{-t/\bar{\tau}})$  to get  $G_{green}(t) = G_U \delta(t) - \Delta G \left( \frac{1}{\bar{\tau}} \right) e^{-t/\bar{\tau}} u(t)$ . From here we write Fourier transform, to get dynamic shear modulus  $\bar{G}(\omega)$  as follows

$$\begin{aligned}G(\omega) &= \mathcal{F} \{ G_{green}(t) \} \\ &= \mathcal{F} \left\{ G_U \delta(t) - \Delta G \left( \frac{1}{\bar{\tau}} \right) e^{-t/\bar{\tau}} u(t) \right\} \\ &= G_U - \frac{\Delta G}{1 + \omega \bar{\tau}} \\ \bar{G}(\omega) &= [G(\omega)]_{\omega \rightarrow -\omega} = G_U - \frac{\Delta G}{1 - \omega \bar{\tau}}\end{aligned}$$

We make a note here that  $G(\omega)$  is also obtained by writing

$$G(\omega) = \frac{1}{J(\omega)} = \frac{1}{J_U + \frac{J_R - J_U}{1 + i\omega\tau}}$$

This we will demonstrate in next section



**Figure-7: The retardation response function shear compliance and relaxation response function shear modulus for a Debye system**

## 29. Electrical Analog of shear modulus-the Electric Modulus

The stress-strain equation (mechanical-system) we have considered is following for a Debye-system

$$\tau \frac{d\gamma(t)}{dt} + \gamma(t) = \tau J_U \frac{d\sigma(t)}{dt} + J_R \sigma(t)$$

The equivalent Electric Field relaxation (retardation) is

$$\tau \frac{d\mathbf{D}(t)}{dt} + \mathbf{D}(t) = \tau \epsilon_\infty \frac{d\mathbf{E}(t)}{dt} + \epsilon_s \mathbf{E}(t)$$

For mechanical system, the retardation function of  $J(t)$  for unit-step of  $\sigma(t)$  input is  $J(t) = J_U + \Delta J(1 - e^{-t/\tau})$  with  $\Delta J = J_R - J_U$ ; similar to that  $J(t)$  we have  $\varepsilon(t)$ , and the retardation response to unit-step of electric field excitation, as

$$\varepsilon(t) = \varepsilon_\infty + \Delta\varepsilon(1 - e^{-t/\tau}); \quad \Delta\varepsilon = \varepsilon_s - \varepsilon_\infty$$

The retardation response curve  $\varepsilon(t)$  is same as that shown in Figure-7, for  $J(t)$ . The similarities of Mechanical and Electrical system is listed in Table-1.

<b>Mechanical System</b>	<b>Electrical System</b>
Stress $\sigma(t)$	Electric Field $\mathbf{E}(t)$
Strain $\gamma(t)$	Displacement $\mathbf{D}(t)$
Shear-Compliance $J(t)$	Permittivity $\varepsilon(t)$
$\gamma(t) = J(t)\sigma(t)$	$\mathbf{D}(t) = \varepsilon(t)\mathbf{E}(t)$
Shear-Modulus $G(t)$	Electric Modulus $M(t)$
$\sigma(t) = G(t)\gamma(t)$	$\mathbf{E}(t) = M(t)\mathbf{D}(t)$
$G(t) = 1/J(t)$	$M(t) = 1/\varepsilon(t)$
Dynamic-Shear-Compliance $J(\omega) = \text{Re}[J(\omega)] + i \text{Im}[J(\omega)]$	Dynamic Permittivity $\varepsilon(\omega) = \text{Re}[\varepsilon(\omega)] + i \text{Im}[\varepsilon(\omega)]$
Dynamic-Shear-Modulus $G(\omega) = \text{Re}[G(\omega)] + i \text{Im}[G(\omega)]$	Dynamic-Electric-Modulus $M(\omega) = \text{Re}[M(\omega)] + i \text{Im}[M(\omega)]$

**Table-1: Mechanical and Electrical System equivalence**

On the similar lines, we can write the relaxation response for Electric Modulus (like shear –modulus), as

$$M(t) = M_\infty - \Delta M(1 - e^{-t/\bar{\tau}}); \quad \Delta M = M_\infty - M_s$$

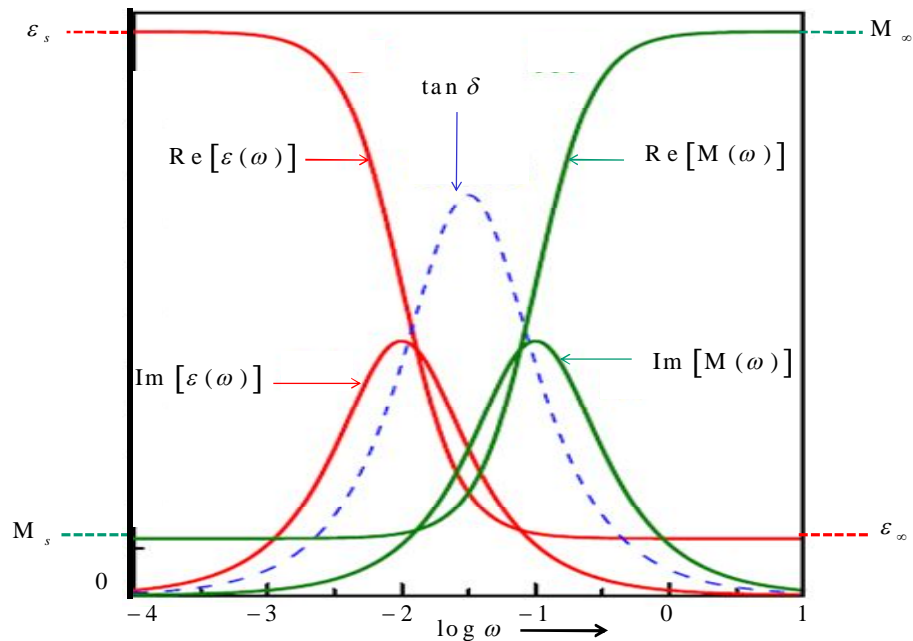
Where  $M_\infty = 1/\varepsilon_\infty$ ,  $M_s = 1/\varepsilon_s$ ,  $\bar{\tau} = (\varepsilon_\infty / \varepsilon_s)\tau$ . We note that  $\bar{\tau} < \tau$ . Similar to  $J(\omega) = J_U + \frac{J_R - J_U}{1 + i\omega\tau}$  obtained via Fourier transformation of Green's function, we write

$$\begin{aligned}
\varepsilon(\omega) &= \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau} \\
M(\omega) &= \frac{1}{\varepsilon(\omega)} = \frac{1}{\varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega\tau}} \\
&= \frac{1 + i\omega\tau}{\varepsilon_\infty(1 + i\omega\tau) + \varepsilon_s - \varepsilon_\infty} = \frac{1 + i\omega\tau}{\varepsilon_\infty i\omega\tau + \varepsilon_s} = \frac{\varepsilon_\infty(1 + i\omega\tau)}{\varepsilon_\infty(\varepsilon_\infty i\omega\tau + \varepsilon_s)} \\
&= \frac{(\varepsilon_\infty i\omega\tau + \varepsilon_s) + \varepsilon_\infty(1 + i\omega\tau) - (\varepsilon_\infty i\omega\tau + \varepsilon_s)}{\varepsilon_\infty(\varepsilon_\infty i\omega\tau + \varepsilon_s)} \\
&= \frac{1}{\varepsilon_\infty} + \frac{(1 + i\omega\tau) - \frac{1}{\varepsilon_\infty}(\varepsilon_\infty i\omega\tau + \varepsilon_s)}{\varepsilon_\infty i\omega\tau + \varepsilon_s} = \frac{1}{\varepsilon_\infty} + \frac{1 - \frac{\varepsilon_s}{\varepsilon_\infty}}{\varepsilon_s + \varepsilon_\infty i\omega\tau} \\
&= \frac{1}{\varepsilon_\infty} + \frac{\frac{1}{\varepsilon_s} - \frac{1}{\varepsilon_\infty}}{1 + i\omega\left(\frac{\varepsilon_\infty}{\varepsilon_s}\tau\right)}; \quad M_\infty = \frac{1}{\varepsilon_\infty}, \quad M_s = \frac{1}{\varepsilon_s}, \quad \bar{\tau} = \frac{\varepsilon_\infty}{\varepsilon_s}\tau \\
M(\omega) &= M_\infty + \frac{M_s - M_\infty}{1 + i\omega\bar{\tau}}
\end{aligned}$$

Experiments which access the quantity  $\varepsilon(\omega)$  are usually termed dielectric relaxation methods, although  $\varepsilon(\omega)$  and  $\varepsilon(t)$  actually refer to dielectric retardation. The true dielectric relaxation, the modulus  $M(t)$  corresponds to the decay of the electric field  $\mathbf{E}(t)$  under the conditions of a constant dielectric displacement  $\mathbf{D}(t) = \mathbf{D}_0(u(t))$ ; or constant charge per area; where  $u(t)$  is unit-step function.

The frequency dispersion curves for dynamic dielectric permittivity  $\text{Re}[\varepsilon(\omega)]$ ,  $\text{Im}[\varepsilon(\omega)]$ , dynamic Electric Modulus  $\text{Re}[M(\omega)]$  and  $\text{Im}[M(\omega)]$  are plotted in Figure-8, for the considered Debye system. The one more significant parameter  $\tan \delta = \text{Im}[\varepsilon(\omega)] / \text{Re}[\varepsilon(\omega)]$  is also shown in Figure-8.

Some of the non-Debye retardation function are  $\varepsilon(t) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty)\left(1 - e^{-(t/\tau)^\alpha}\right)$  with  $0 < \alpha < 1$ ,  $\varepsilon(t) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty)\left(1 - E_\alpha(-(t/\tau)^\alpha)\right)$ , where  $E_\alpha(-x^\alpha)$  is one parameter Mittag-Leffler function, plus many others can be constructed. Similarly non-Debye dynamic dielectric permittivity can be formulated as Cole-Cole type, i.e.  $\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + (i\omega\tau)^\beta}$  or Cole-Davidson type i.e.  $\varepsilon(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{(1 + i\omega\tau)^\gamma}$ , and several others type. Nonetheless the point to be mentioned that any type of relaxation or retardation, (simple Debye, complex non-Debye type) where the dynamic susceptibility is evaluated or experimentally found, needs to satisfy Kramer-Kronig relation and thus need be causal.



**Figure-8: Frequency Dispersion curves for dynamic dielectric permittivity and dynamic Electric Modulus**

### 30. Conclusions

In this lecture note, what we have discussed a universal known phenomena causality that is the response (effect) comes only after cause. This simple universal phenomenon has associated mathematics especially in complex-analysis, otherwise looks very complicated, that we have described and simplified. The major outcome of causal systems are Kramer-Kronigs relations, that we have derived and described its utility in practical systems. We have described several examples and noted especially the Debye relaxation (retardation) phenomena in time domain and then in frequency domain. The theories described here can be applied to non-Debye systems, that are complex relaxation or retardation phenomena of system responses, however, the principles of causality still be maintained. We have considered response functions of the causal systems to be continuous and mainly differentiable every-where. The mathematics of causality of the system response function, which is continuous but nowhere differentiable, is yet not developed. That is a separate research all together.

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