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Linear Response Theory

1 Definition of response function χ

The relation $\delta\langle M\rangle = \langle M\rangle - M_0 = \chi H$ relates a response $\delta\langle M\rangle$ to an applied external field H. In case there is a magnetization $\langle M\rangle = M_0$ in zero applied field, this has been subtracted out. This defines a linear response coefficient χ. Since the complete response will always have some non-linear behavior at high fields H, it is necessary to remember that χ is defined in the limit of a small applied field ($\chi = \partial\langle M\rangle/\partial H$.) It is also assumed that the system is held close to thermal equilibrium at temperature T by a heat bath.

Here is the generalization to a general response to an arbitrary field $F(\vec{r},t)$. Ordinarily the response is a measureable property $x(r)$, the expectation value of an operator $\hat{x}(r)$. The general linear relation between $x(r)$ and F is

$$\delta x(\vec{r},t) = \delta\langle\hat{x}(\vec{r},t)\rangle = \int d\vec{r}' \int_{-\infty}^{\infty} dt' \chi(\vec{r},\vec{r}';t-t')F(\vec{r}',t'). \tag{1}$$

Note that the response in general can be non-local in space and in time. The range in time over which the system "remembers" the earlier external perturbation is the characteristic relaxation or thermalization time τ. (Hydrodynamic effects can cause long-time "tails" in the response function, which are unimportant for transport properties of solids.) The spatial range is either the range of the screened particle-particle or particle-probe interaction, or else the particle mean free path or thermalization length ℓ.

To simplify notation, the rest of these notes will suppress the space dependence and work only with the time-dependence.

$$\delta x(t) = \int_{-\infty}^{\infty} dt' \chi(t-t')F(t') \tag{2}$$

2 Causality

While in equilibrium, the system is invariant in time (this is the definition of equilibrium.) 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 field acts. Before the field F is applied, there can be no response (this is the "principle of causality.") Suppose the field has the form of a "unit impulse", $F(t) = \delta(t)$. From Eq. (2), the response to this unit impulse is

$$\delta x(t) = \chi(t) \tag{3}$$

To say it in words, $\chi(t)$ is the response at time t to a unit impulse applied at time $t = 0$. By the principle of causality, $\chi(t)$ must be zero for negative times t.

It is also interesting to consider the response to an *ac* applied field

$$F(t) = F_0 e^{-i\omega t} \tag{4}$$

$$\delta x(t) \equiv \chi(\omega) F_0 e^{-i\omega t}. \tag{5}$$

This defines the frequency-dependent susceptibility, $\chi(\omega)$. From Eqs. (2,4,5) and causality, we find

$$\chi(\omega) = \chi_1 + i\chi_2 = \int_0^\infty d\tau \chi(\tau) e^{i\omega\tau}. \tag{6}$$

Thus $\chi(\omega)$ is a complex function. Any actual applied field $F(t)$ will be a real quantity, so the correct interpretation of Eq. (4) is that only the "real part" $F_0 \cos(\omega t)$ is meant. Because the response is linear, and taking the real part is a linear operation, therefore the response to the real part of the complex field $F_0 \cos(\omega t)$ is the real part of the (not actually physical) response to the complex field. This means that the correct interpretation of Eq. (5) is

$$\delta x(t) = \chi_1(\omega) F_0 \cos(\omega t) + \chi_2(\omega) F_0 \sin(\omega t). \tag{7}$$

Thus the "real" and "imaginary" parts χ_1 and χ_2 have the interpretations that χ_1 gives the "in-phase" part of the response (oscillating like $\cos(\omega t)$ as does the field) while χ_2 gives the "out-of-phase" response. It will turn out that one of these parts contains the dissipative response, and the other is "reactive."

Causality gives an important relation between these two pieces, known as the "Kramers-Kronig" relations. First we show that causality implies that $\chi(\omega)$ as given in Eq. (6), is analytic in the upper half of the complex z plane, when considered as a function of a complex frequency z (whose real part is the physical frequency ω.) Writing $z = x + iy$ where $x = \omega$,

$$\chi_1 = \int_0^\infty d\tau \chi(\tau) e^{-y\tau} \cos(x\tau) \tag{8}$$

$$\chi_2 = \int_0^\infty d\tau \chi(\tau) e^{-y\tau} \sin(x\tau). \tag{9}$$

The Cauchy relations are necessary and sufficient conditions for a function to be analytic, and are clearly satisfied by Eqs. (8,9):

$$d\chi_1/dx = d\chi_2/dy \tag{10}$$

$$d\chi_2/dx = -d\chi_1/dy. \tag{11}$$

To prove that Eqs. (10,11) follow from (8,9) it is necessary to interchange the operations of differentiation and integration, which is permitted only if the integrals are absolutely convergent. This property clearly holds only when $y > 0$, *i.e.* in the upper half z plane. Also it is clear that if χ had not been causal, that is, if $\chi(\tau)$ had been non-zero for negative as well as positive times τ, then analyticity would not have been established anywhere. The fact that it is the **upper** rather than the lower half of the complex frequency plane where χ is analytic follows from an arbitrary sign convention introduced in Eq. (4), namely that the external field oscillates as $e^{-i\omega t}$ rather than as $e^{+i\omega t}$. The two choices are equally sensible, so it is necessary to choose a convention and stick with it.

The Kramers-Kronig relations are valid for any function which is analytic in the upper half plane and vanishes as $|z| \to \infty$. Cauchy's theorem gives the identity

$$0 = \oint_C dz \frac{\chi(z)}{z - \omega} \tag{12}$$

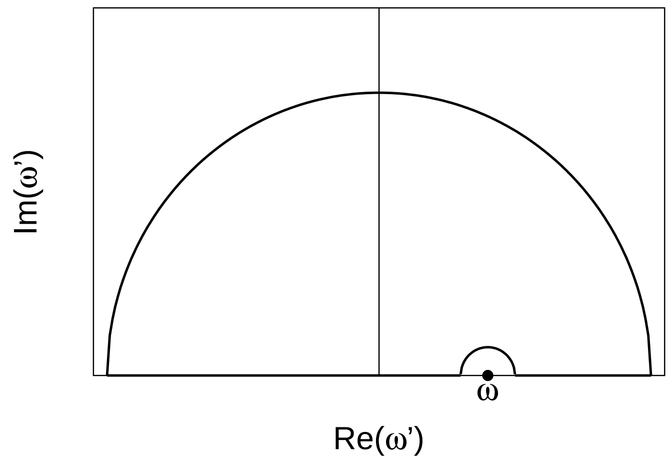

Figure 1: Contour C for Eq. (12 – Kramers-Kronig relation

where C could be any contour confined to a region where $\chi(\omega)$ is analytic, and not containing the point $z=\omega$. Let C denote the contour shown in fig.1. Because χ vanishes as $|z|$ goes to infinity, the large arc of C contributes nothing as it recedes to infinity. The remaining part of the contour can be separated into the straight part along the real axis, which becomes a principle-value integral as the small arc shrinks, and an integral over the small arc which is parameterized by $z=\omega+\epsilon e^{i\phi}$. Thus Eq. (12) becomes

$$0 = P\int_{-\infty}^{\infty} d\omega' \frac{\chi(\omega')}{\omega'-\omega} + \lim_{\epsilon\to 0}\int_{\pi}^{0} \frac{i\epsilon e^{i\phi}d\phi}{\epsilon e^{i\phi}}\chi(\omega+\epsilon e^{i\phi}). \tag{13}$$

This becomes the general relation

$$\chi(\omega) = \frac{P}{i\pi}\int_{-\infty}^{\infty} d\omega' \frac{\chi(\omega')}{\omega'-\omega}. \tag{14}$$

Finally, separating into real and imaginary parts and using the results from Eqs. (8,9) that χ_1 is even in ω and χ_2 is odd, this becomes

$$\chi_1(\omega) = \frac{2P}{\pi}\int_0^{\infty} d\omega' \frac{\omega'\chi_2(\omega')}{\omega'^2-\omega^2} \tag{15}$$

$$\chi_2(\omega) = -\frac{2\omega P}{\pi}\int_0^{\infty} d\omega' \frac{\chi_1(\omega')}{\omega'^2-\omega^2}. \tag{16}$$

3 Damped Harmonic Oscillator

The Harmonic oscillator is the canonical example. The quantum results are essentially the same as the classical results, so consider the Newtonian equation

$$m\ddot{x} + m\dot{x}/\tau + m\omega_0^2 x = F(t) \tag{17}$$

where $1/\tau$ is a phenomenological damping rate, and $m\omega_0^2$ is the spring constant K. If $F(t)$ has only a single Fourier component $F_0\exp(-i\omega t)$, then $\delta x(t)$ is $\chi(\omega)F_0\exp(-i\omega t)$, and one gets

$$\chi(\omega) = \frac{-1/m}{\omega^2+i\omega/\tau-\omega_0^2} = \frac{-1/m}{(\omega-\omega_1)(\omega-\omega_2)} \tag{18}$$

$$\omega_{1,2} = -i/2\tau \pm \tilde{\omega} \tag{19}$$

$$\tilde{\omega} = \sqrt{\omega_0^2 - 1/4\tau^2} \tag{20}$$

Note that the response function has two simple poles, at ω_1 and ω_2, both in the lower half of the complex plane.

Now calculate $\chi(t)$ by Fourier inversion,

$$\chi(t) = \frac{-1}{2\pi m} \int_{-\infty}^{\infty} \frac{d\omega e^{-i\omega t}}{(\omega - \omega_1)(\omega - \omega_2)}. \tag{21}$$

The factor $\exp(-i\omega t)$ decays to zero when ω is continued to complex values, provided the upper half ω-plane is used for $t < 0$ and the lower half plane for $t < 0$. We then convert the line integral in Eq. 21 into a closed contour integral by adding the distant arc in the appropriate half plane which contributes nothing as it recedes to infinity. Since the integrand for $t < 0$ is analytic in the upper half plane, the answer is $\chi(t) = 0$ for $t < 0$ as it must be by causality. For $t > 0$, the contour encloses the two poles in the lower half plane, so by Cauchy's theorem the value is $-2\pi i$ times the sum of the two residues, or

$$\chi(t) = \frac{1}{m\tilde{\omega}} e^{-t/\tau} \sin(\tilde{\omega} t)\theta(t). \tag{22}$$

This is the response to the unit impulse at t=0. Sinusoidal oscillations begin at $t = 0$ with zero amplitude and unit momentum $m\dot{x}(0) = 1$. The distance $1/2\tau$ of the poles from the real axis determines the damping rate. The real part of the location of the pole fixes the oscillation frequency $\tilde{\omega}$. These canonical results serve as a model for the behavior of response functions in general.