linear-response.

Suppose we are interested in quantity $x$, which is zero in the
eq. state, and would like to know $\langle x \rangle \neq 0$ in response to the
external perturbation

$$V(t) = -x \cdot f(t)$$

applied. Call $f(t)$ a generalized force; it may explicitly depend
on time. Before deriving the quantum-mechanical expression,
for $\langle x \rangle$, we will establish some general properties of the
response function which any equil. system in nature must obey

The linear response $\langle x(t) \rangle$ at time $t$ depends on the
applied field at all preceding moments in time

$$\langle x(t) \rangle = \int_0^\infty \chi(\tau) f(t-\tau) d\tau,$$

where the generalized susceptibility $\chi(\tau)$ is the property
of the system state. (Since $f \to 0$ we care only about

In the Fourier representation this Eq. reads

$$\langle x \rangle_\omega = \omega \cdot \chi_\omega$$
where \( d(w) = \int_0^\infty \hat f(t) e^{i\omega t} dt \) (in other words \( \langle x \rangle_\omega \) is the response to the monochromatic perturbation \( f(t) = f_\omega e^{i\omega t} \)). The beauty of the consideration presented below is in how much knowledge can be obtained by pure reasoning and math. Formally \( d\omega \) is complex

\[
d\omega = d\omega' + i d\omega''
\]

The definition of \( d\omega \) immediately tells us that by complex conjugation of the time integral we obtain \( d(-\omega) \), thus

\[
d(-\omega) = d^*(\omega) \Rightarrow d(-\omega) + i d''(-\omega) = d(\omega) - i d''(\omega)
\]

i.e. real part is an even function of \( \omega \), and the imaginary part is odd:

\[
d'(\omega) = d'(-\omega) ; \quad d''(\omega) = -d''(-\omega)
\]

It means that when \( \omega \to 0 \)

\( \alpha'' \) has to go to 0 or to diverge

\[
\begin{array}{c|c}
\quad & \text{Function} \\
\hline
\omega & d\omega' \\
\hline
\omega & d\omega'' \\
\end{array}
\]

Next, none system may respond to the infinitely fast oscillating force. From this we deduce that \( d(\omega) \to 0 \) as \( |\omega| \to \infty \).

When external time-dependent perturbation is applied to the system it causes transitions between the energy levels (classically, it accelerates/deaccelerates particles) and thus is accompanied by the absorption/dissipation of energy which is ultimately converted into heat. To find heat dissipation we write

\[
\frac{dE(t)}{dt} = \frac{d}{dt} \langle \psi(t) | \hat H(t) | \psi(t) \rangle = \langle \psi | \frac{d}{dt} \hat H | \psi \rangle + \langle \psi | \hat H(t) | \psi \rangle + \langle \psi | \frac{d}{dt} \hat H | \psi \rangle = -i \langle \psi | \hat H | \psi \rangle + i \langle \psi | \hat \psi \rangle + \langle \psi | \hat v \rangle
\]

i.e.

\[
E = -\langle x(t) \rangle^2
\]

(sometimes this expression may be used to find the general force).
Substituting here \( \xi(\omega) \) from the linear response relation we find for the external force \( f = \frac{1}{2} \left( f_0 e^{-i\omega t} + f_0^* e^{i\omega t} \right) \)

\[
\dot{E} = Q_\omega = -\frac{i}{4} \left( \omega f_0 e^{-i\omega t} + \omega^* f_0 e^{i\omega t} \right) (-i\omega) \left( f_0 e^{-i\omega t} + f_0^* e^{i\omega t} \right)
\]

After averaging over the period of one oscillation, \( \frac{\omega}{2\pi} \int_0^{2\pi/\omega} \dot{E} \, dt \), we establish the link between the dissipated heat and the imaginary part of \( \xi \)

\[
Q_\omega = \frac{1}{4} (-i\omega \omega^* + i\omega^* \omega) \left| f_0 \right|^2 = \frac{1}{2} \omega \xi''(\omega) \left| f_0 \right|^2
\]

(terms \( e^{-2i\omega t} \) contribute zero after averaging over the period). Any physical processes disturbing the system result in the energy dissipation, thus \( Q_\omega \) must be positive. It means that \( \xi''(\omega) \) is positive and non-zero for all \( \omega > 0 \).

Next we consider \( \xi(\omega) \) as a function of complex variable \( \omega = \omega' + i\omega'' \) (of course, only real \( \omega \) are physically meaningful). Since \( \xi(t) \) is finite for all positive \( t \) we conclude that \( \xi(\omega) \) is a single-valued function everywhere in the upper half-plane. Indeed:

\[
\int_0^\infty e^{i\omega' t} - \omega''^t \xi(t) \, dt = \text{well behaved and convergent for } \omega'' > 0;
\]

thus no branch-cuts or poles are possible. Since any system "forgets" its own history with some characteristic time-scale, \( \xi(t) \) must vanish in the limit of \( t \to \infty \). It follows then that on a real axis \( \xi(\omega) \) is defined by the convergent integral and thus has no singularities at \( \omega'' = 0 \), except, possibly, at \( \omega = 0 \). All these nice properties follow from the fact that the integration is from \( t=0 \) to \( t=\infty \), also known as a "casualty principle" - past determines future, not otherwise.

The other property of interest is

\[
\xi^*(-\omega^*) = \xi(-\omega) \quad \text{a generalization of} \quad \xi^*(\omega) = \xi(-\omega) \quad \text{to the complex } \omega \text{ case.}
\]
If \( w \) is purely imaginary we get \( d^*(i\omega) = d(i\omega) \), i.e. \( d \) is real on the imaginary axis. We are not done yet!

Consider the integral

\[
\frac{1}{2\pi i} \int_C \frac{dd(w)}{dw} \frac{dw}{d(w) - a}
\]

taken around contour \( C \) with real \( a \). Since \( d(w) \) has no poles inside \( C \), the integral equals to the number of zeros of \( d(w) - a \). On another hand we write it as

\[
\frac{1}{2\pi i} \int_{C'} \frac{dd}{d - a}
\]

where \( C' \) is the map of \( C \) on the \( d \)-plane. The infinite semi-circle maps to \( d = 0 \). The \( \omega = 0 \) point maps to some real value \( \lambda_0 \) (in some cases \( \lambda_0 = \infty \)). [We expect \( \lambda_0 \geq 0 \) because in response to the static \( v = -xf_0 \) with \( f_0 > 0 \), the system will go to the state with lower energy by developing \( \langle x \rangle = x_0 f_0 \) with positive \( x_0 \).] Finally the real \( \omega > 0 \) and \( \omega < 0 \) lines map to some complicated lines with \( d'' > 0 \) if \( \omega > 0 \) and \( d'' < 0 \) if \( \omega < 0 \), i.e. there are no other intersections of \( C' \) with real \( d \)-axis except at \( d = 0 \) and \( d = \lambda_0 \).

The structure of \( C' \) suggests that our integral is non-zero and equals unity if, and only if, \( \partial A < \lambda_0 \). This result transforms into the statement that \( d(\omega) = \lambda = (\text{some real value}) \) only once in the upper half-plane, and only if \( \omega \in (0, \lambda_0) \). On imaginary axis \( d(\omega) \) is real with \( d(0) = \lambda_0 \) and \( d(i\omega \to \infty) = 0 \). The only conclusion is then that \( d(i\omega) \) is a monotone function of \( \omega \), and \( d''(\omega) \neq 0 \) everywhere in the upper
half-plane except the imaginary axis. And further on (!!) this means that \( \phi(w) \) has no zeros in the upper half-plane (with exception of \( w=0 \)).

The following figure summarizes the above mentioned properties:

![Real monotonically increasing function with no singularities or zeros in the upper half-plane](image)

Notice, we know nothing yet what is the system under discussion, and our initial knowledge was close to none, just \( X(t) = \int_{-\infty}^{\infty} \phi(t) \phi(t-\tau) d\tau \)

More properties: Consider the integral

\[
\int_{C} \frac{\phi(w)}{w-w_0} \, dw = 0
\]

Since \( \phi(w) \to 0 \) as \( w \to \infty \) the integral over the infinite semi-circle is zero. The real axis part consists of the principal part integrals over \( w \) and the infinitesimal semi-circle integral around \( w_0 \) (assume \( \omega_0 \) finite). Then

\[
\int_{-\infty}^{w_0} \frac{\phi}{w-w_0} \, dw + \int_{w_0}^{\infty} \frac{\phi}{w-w_0} \, dw - i\pi \phi(w_0) = 0
\]

or

\[
\int_{-\infty}^{\infty} \frac{\phi(z)}{z-w} \, dz = i\pi \phi(w)
\]

Substituting \( \phi = \phi' + i\phi'' \) and using even/odd symmetry of \( \phi' \) and \( \phi'' \) we obtain

Kramers-Kronig relations

\[
\begin{aligned}
\phi' &= \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\phi''(z)}{z-w} \, dz \quad ; \quad \phi'' = -\frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\phi'(z)}{z-w} \, dz \\
\phi' &= \frac{2}{\pi} \int_{0}^{\infty} \frac{z \phi''(z)}{z^2-w^2} \, dz \quad ; \quad \phi'' = -\frac{2w}{\pi} \int_{0}^{\infty} \frac{\phi'(z)}{z^2-w^2} \, dz
\end{aligned}
\]
If \( d(\omega) \) has a pole at \( \omega = 0 \) of the form \( d(\omega) = \frac{\omega^2}{\omega} \), then we have to modify these relations by adding \( A/\omega \) to the imaginary part

\[
\alpha'' = -\frac{2\omega}{\pi} \int_0^\infty \frac{\omega^2}{\omega^2 - \omega^2} d\omega + \frac{A}{\omega}
\]

All of this is heavily used since different experimental techniques measure different \( \omega \)-regions, some of them look at \( \omega'' \), some at \( \omega' \).

The final relation which is quite useful in some cases expresses \( \alpha''(\text{real } \omega) \) in terms of \( \alpha''(\text{imaginary } \omega) \) measured ('the easiest to calculate theoretically using finite-\( T \) diagrammatic methods')

Consider

\[
\int_C \frac{\omega d(\omega)}{\omega^2 + \omega^2} d\omega = \int_C \frac{2d(\omega)}{\omega^2 + \omega^2} d\omega = i\pi d(i\omega),
\]

i.e.

\[
d(i\omega) = \frac{2}{\pi} \int_0^\infty \frac{\omega d''(\omega)}{\omega^2 + \omega^2} d\omega
\]

In particular

\[
\int_0^\infty d(i\omega) d\omega = \int_0^\infty d''(\omega) d\omega
\]

Unfortunately, not the other way around

\[
d''(\omega) = \cdots \text{ on imaginary axis}
\]