Linear response theory

Consider a many-body problem with Hamiltonian $H_0$ which is perturbed by an external probe

$$\hat{H} = H_0 + \int_0^t \hat{A} \, dt$$

where $\hat{A}$ is a time-dependent operator.

Examples:

<table>
<thead>
<tr>
<th>$E_i$</th>
<th>$B$</th>
<th>$g_{ij}$</th>
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</thead>
<tbody>
<tr>
<td>$\hat{A}$</td>
<td>$\hat{A}$</td>
<td>$\hat{A}$</td>
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<tr>
<td>$\hat{n}$</td>
<td>$\hat{j}_i$</td>
<td>$\hat{n}$</td>
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If the probe is weak, the structure of the state is perturbed only slightly, and we can derive the linear response relation for the evolution of $\hat{B}(t)$:

$$\hat{B}_n(t) = \hat{O}^+(t) \hat{B}(t) \hat{O}(t) \quad \text{for} \quad \hat{B}(t; k_0)$$
\[ O(t) = T \exp \left( -i \int_0^t \hat{A}_I(t') f(t') \right) \]
\[ \approx 1 - i \int_0^t \hat{A}_I(t') f(t') + \Theta(t^2) \]
\[ \hat{B}_H(t) = \hat{B}_I(t) - i \int_0^t \left[ \hat{B}_I(t'), \hat{A}_I(t') \right] f(t') \]

In the good thermal state
\[ \langle \delta B(t) \rangle = \int_0^\infty dt' \chi_{BA}^k(t, t') f(t') \]
where the retarded response function
\[ \chi_{BA}^k(t-t') = -i \left\langle \left[ \hat{B}_I(t), \hat{A}_I(t') \right] \right\rangle \theta(t-t') \]

- \( \Theta(t-t') \) follows from causality
- \( \chi_k \) is an intrinsic property of the unperturbed system
- In Fourier space
\[ \langle \delta B(\omega) \rangle = \chi(\omega) f(\omega) \]
- Often \( \hat{A} = \hat{B} \) - lets restrict it now
Consider a thermal state

\[ \langle \hat{\Theta} \rangle = \frac{\text{Tr} \left( \Theta e^{-\beta \hat{H}_0} \right)}{\text{Tr} \left( e^{-\beta \hat{H}_0} \right)} \]

Using now the full basis of eigenstates \( \hat{H}_0 |\alpha\rangle = E_{\alpha} |\alpha\rangle \)
we can express the Fourier transformed correlation function

\[ \chi^R(t, t') = -i \langle [\hat{A}(t), \hat{A}(t')] \rangle \theta(t-t') \]

\[ e^{i\beta t} \hat{A} e^{-i\beta t} \]

\[ \chi^E(\omega) = Z^{-1} \sum_{a,b} \left( e^{-E_a / T} - e^{-E_b / T} \right) \frac{\langle a | \hat{A} | b \rangle \langle b | \hat{A} | a \rangle}{\omega + E_{a-b} + i 0^+} \]

where \( E_{a-b} = E_a - E_b \)

This is the Lehmann spectral decomposition
We can relate it to the time-ordered imaginary-time correlation function

\[ \chi^\tau(\tau, \tau') = - \langle T_{\tau} \hat{A}(\tau) \hat{A}(\tau') \rangle \]

where \( \hat{A}(\tau) = e^{\tau H_0} \hat{\mathcal{A}} e^{-\tau H_0} \) at \( \tau = 0 \leq \tau, \tau' \leq \beta = 1/T \to \text{compact} \) and the time ordering is defined

\[ \mathcal{T} \hat{A}(\tau) \hat{A}(\tau') = \left\{ \begin{array}{ll} \hat{A}(\tau) \hat{A}(\tau') & \tau > \tau' \\ \hat{A}(\tau') \hat{A}(\tau) & \tau < \tau' \end{array} \right. \]

Since \( \tau \) is periodic \( \tau = \tau + \beta \)

\[ \chi^\tau(\tau') = \sum_{\eta} e^{i \omega_n \tau} \chi^\tau(i\omega_n) \]

Matsubara frequencies \( \omega_n = 2\pi n T \)

we now decompose:

\[ \chi^\tau(i\omega_n) = Z^{-1} \sum_{a, b} \left( e^{-E_a / T} - e^{-E_b / T} \right) \frac{\langle a | \hat{A} | b \rangle < b | \hat{A} | a \rangle}{i\omega_n + E_{ab}} \]
If we now compare spectral representations of $\chi(\omega)$ and $\chi(i\omega)$:

$$\chi(\omega) = \chi(i\omega) \quad (i\omega \rightarrow \omega + i0^+)$$

This suggests the following strategy to compute response function $\chi(\omega)$:

1) First compute $\chi(i\omega)$, this can be done diagramatically or using functional integration.

2) Perform analytic continuation $i\omega \rightarrow \omega + i0^+$. Given an analytical expression for $\chi(i\omega)$, this is very easy. If $\chi(i\omega)$ is known only numerically, analytic continuation is tricky.
Example: longitudinal conductivity of a metal (As)

Consider a time-dependent electric field $\vec{E}(t)$ that induces the current $\vec{j}(t)$. In the absence of time-reversal breaking (e.g., magnetic field)

$$\vec{j}(\omega) = \sigma(\omega) \vec{E}(\omega)$$

\[\text{longitudinal AC conductivity}\]

In 1900 Drude proposed a classical calculation of the AC conductivity:

$$m \ddot{\vec{v}}_i = -e \vec{E}_i - \frac{m}{\tau} \dot{\vec{v}}_i$$

Introducing the velocity $\dot{\vec{v}}_i = \vec{u}_i$

$$-i m \omega \vec{u}_i(\omega) = e \vec{E}_i(\omega) - \frac{m}{\tau} \vec{u}_i(\omega)$$

$$\vec{u}_i(\omega) = \frac{-e \vec{E}_i(\omega)}{m (-i \omega + \frac{1}{\tau})}$$
and the current $j_i = -e n v_i$ is

$$j_i(\omega) = \frac{ne^2}{m} \frac{1}{\tau - i\omega} E_i(\omega)$$

ballistic regime Drude AC conductivity

$\omega \gg \tau^{-1}$  \(\sigma(\omega) \approx \frac{ne^2}{m} \frac{1}{\omega}\)

$\omega \ll \tau^{-1}$  \(\sigma(\omega) \approx \frac{ne^2\tau}{m} \rightarrow \text{steady current}\)

But the world is governed by quantum mechanics, can we check Drude's classical prediction against QM linear response calculation?

**Electromagnetic linear response**

Consider linear response of electromagnetic current \(j_{\mu}\) to external gauge potential \(A_\mu\): \(\mu, \nu = t, x, y, z\)

$$\langle j_{\mu}(x) \rangle = \int d x' K_{\mu\nu}(x, x') A_\nu(x')$$
General properties of $k_{\mu \nu}(x, x')$:

- Pure gauge cannot induce current

$$0 = \int d^4 x' \ k_{\mu \nu}(x, x') \partial^\alpha \ f(x') = \int d^4 x' k_{\mu \nu}(x, x') \partial^\alpha \ f(x')$$

- Current must be conserved

$$\partial^\mu j^\mu(x) = \int d^4 x' \partial^\mu k_{\mu \nu}(x, x') \ A^\nu(x')$$

How to compute $k_{\mu \nu}(x, x')$?

First we can get the current

$$\delta S \sim \int \partial^\mu j^\mu \ \delta A^\mu - \text{Noether current}$$

and since $A^\mu \rightarrow A^\mu + \partial^\mu \phi$

$$j^\mu = \frac{\delta S[A]}{\delta A^\mu}$$

The expectation value $\langle j^\mu \rangle$ can be extracted from logarithm of

$$Z[A] = \int D\phi \ e^{-S[\phi, A]}$$

define $W[A] = -\log Z[A]$
\[
\langle j^\mu \rangle = \frac{\delta W[A]}{\delta A^\mu} = \frac{\int D\phi \frac{\delta S}{\delta A_\mu} e^{-S}}{Z}
\]

So by construction,

\[
K_{\rho\sigma}(x,x') = \frac{S^2 W[A]}{\delta A_\mu(x) \delta A_\nu(x')}
\]

\[
= \frac{\int D\phi \frac{\delta S}{\delta A_\mu} \frac{\delta S}{\delta A_\nu} e^{-S}}{Z^2} - \frac{\int D\phi \frac{\delta S}{\delta A_\mu} \frac{\delta S}{\delta A_\nu} e^{-S}}{Z^2}
\]

\[
+ \frac{\int D\phi \frac{\delta S}{\delta A_\mu} \frac{\delta S}{\delta A_\nu} e^{-S}}{Z^2} \frac{\int D\phi \frac{\delta S}{\delta A_\nu} \frac{\delta S}{\delta A_\mu} e^{-S}}{Z^2}
\]

\[
= \left\langle \frac{S^2 S}{\delta A_\mu(\delta S) A_\nu(\delta S)} \right\rangle - \left\langle j^\mu(x) j_\nu(x') \right\rangle
\]

\[
\text{diagonal term}
\]

\[
\text{paramagnetic term}
\]

\[
Kubo formula
\]
As example, we sketch the Euclidean effective theory of Goldstone bosons: $A_0 = i \phi$

$$S[\Theta; A; \phi] = \int d^4 x \frac{n_s}{2m} \left[ \frac{1}{c_s^2} (\partial_\tau \Theta)^2 + (\partial_i \Theta)^2 \right]$$

where $\partial_\tau \Theta = \partial_\tau \Theta - \phi$; $\partial_i \Theta = \partial_i \Theta - A_i$.

Let's compute the conductivity

$$j_i (\omega, q) = \sigma (\omega, q) E_i (\omega, q)$$

$$\sigma (\omega, q) = \frac{1}{\omega} K_{ii} (\omega, q) \mid_{\omega \to -\omega}$$

We now compute $K_{ij} (\omega, q)$ for the effective theory:

$$j_i = \frac{\delta S}{\delta A_i} = -\frac{n_s}{m} \partial_\tau \Theta$$

$$\frac{\delta S}{\delta A_i \delta A_j} = \frac{n_s}{m} \delta_{ij}$$
$k_{ij}(x,x') = \frac{\hbar s}{m} \left( \delta_{ij} - \frac{\hbar s}{m} \langle \theta_i \theta_j \rangle \right)$

Diagrammatically

In momentum space

$\langle \theta_q \theta_{-q} \rangle = -\frac{m}{\hbar} \frac{\omega^2}{(\omega^2 + q^2)}$

$k_{ij}(\omega, q) = \frac{\hbar s}{m} \left( \delta_{ij} - \frac{q_i q_j}{(\omega^2 + q^2)} \right)$

$= \frac{\hbar s}{m} \delta_{ij} \left( \frac{\omega^2}{C_s^2 + q^2} \right) - q_i q_j \frac{\omega^2}{C_s^2 + q^2}$

Imagine we switch on a perturbed $x$-dim

$q_i = (q, 0)$

$k_{xx}(\omega, q) = \frac{\hbar s}{m} \frac{\omega^2}{\omega^2 + C_s^2 q^2}$

After analytic continuation:

$\sigma = \frac{1}{\omega} \left| k_{xx}(\omega - i\omega, q) \right|_{\omega \rightarrow \omega + i\omega}$

$= \frac{\hbar s}{m} \frac{i\omega}{\omega^2 - C_s^2 q^2}$
AC conductivity $\sigma = 0$

$$\sigma(\omega) = \frac{n_s}{m} \frac{i}{\omega + i\alpha_0} = \frac{n_s}{m} \left( \frac{1}{\omega} - i\alpha_0 \right)$$

The real part behaves as $\Re(\omega)$ since we did not introduce disorder which gives rise to a finite $\omega$.

A calculation of $\sigma(\omega)$ in the presence of disorder starting from the microscopic fermion theory can be found e.g. in Altland and Simons or Coleman books.

Main steps:

1. Paramagnetic term $p$

$$\kappa_{\mu \nu}(x, x') = -\frac{i}{m} \langle \hat{\sigma}(x) \rangle \delta(x-x') \delta_{\mu \nu} (1 - \delta_{\rho \sigma})$$

2. Diamagnetic term $\delta$

$$\langle j^\mu(x) j^\nu(x) \rangle$$

Averaging is done

1) over disorder potential

2) over state (e.g. GS or thermal)
Drude metal

\[ \sigma(\omega) = \frac{\hbar e^2}{m} \frac{1}{\omega^2 - i\omega} \]

Let's compute an integral

\[ \int_0^\infty \text{d}\omega \ \text{Re} \ \sigma(\omega) = \int_0^\infty \text{d}\omega \ \frac{\omega^{-2}}{\omega^{-2} + \omega^2} \cdot \frac{\hbar e^2}{m} \]

\[ = \frac{\pi \hbar e^2}{2} \]

Consider now a superconductor

\[ \sigma(\omega) = \frac{\hbar e^2}{m} \frac{i}{\omega + i\delta} \]

\[ \int_0^\infty \text{d}\omega \ \text{Re} \ \sigma(\omega) = \frac{\hbar e^2}{m} \frac{\pi \hbar}{2} \]

The integral is independent of the system. The sum rule measures charge density.
To prove it, consider an electric pulse \( E(t) = E_0 \delta(t) \)

\[
\int_{t_S}^{t} j(t) \, dt = ne \sigma(t_S) = \frac{ne^2 E_0}{\hbar}
\]

\[
\sigma(t_S) E_0 = \sum_{\omega} \int_{-\infty}^{+\infty} e^{-i\omega S} \sigma(\omega) = \frac{ne^2}{\hbar} E_0
\]

Substituting this into the previous expression proves the first rule.
Different systems have the AC weight distributed differently.