Linear response theory

Felix Clavientus

Consider a many-body problem with Hamiltonian $\hat{H}_0$ which is perturbed by an external probe

$$\hat{H} = H_0 + \underset{\substack{\uparrow \\ \text{time-dependent} \\ \text{force}}}{f}(t)\,\hat{A} \rightarrow \text{operator}$$

Examples:

f	ϕ	E_i	B	g_{ij}
$\hat{A}$	$\hat{n}$	$\hat{j}_i$	$\hat{m}$	$\hat{T}_{ij}$

If the probe is weak, the structure of the state is perturbed only slightly and we can derive linear response relations for time-evolution of $\hat{B}(t)$:

$$\hat{B}_H(t) = \hat{U}^+(t)\,\underset{\substack{\| \\ B(t;\,H_0)}}{\hat{B}(t)}\,\hat{U}(t)$$

$$\hat{U}(t) = T\exp\left(-i\int_{-\infty}^{t} dt'\, \hat{A}_I(t) f(t)\right)$$

$$\cong 1 - i\int_{-\infty}^{t} dt'\, \hat{A}_I(t') f(t') + \mathcal{O}(f^2)$$

$$\hat{B}_H(t) = \hat{B}_I(t) - i\int_{-\infty}^{t} dt'\, [\hat{B}_I(t), \hat{A}_I(t')] f(t')$$

In the ground or thermal state

$$\boxed{\langle \delta B(t)\rangle = \int_{-\infty}^{+\infty} dt'\, \underbrace{\chi^R_{BA}(t,t')}_{\text{depends only on } t-t'} f(t')}$$

where the retarded response function:

$$\chi^R_{BA}(t-t') = -i\langle[\hat{B}_I(t), \hat{A}_I(t')]\rangle\theta(t-t')$$

- $\theta(t-t')$ follows from causality
- χ_R 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 to it now

Consider a thermal state

$$\langle \hat{O} \rangle = \frac{\mathrm{Tr}\left(O e^{-\beta \hat{H}_0} \right)}{\underbrace{\mathrm{Tr}\left(e^{-\beta \hat{H}_0} \right)}_{Z}}$$

Using now the full basis of eigenstates $\hat{H}_0 |a\rangle = E_a |a\rangle$

we can express the Fourier transform of retarded correlation function

$$\chi^R(t-t') = -i \langle [\underbrace{\hat{A}(t)}_{e^{+i\hat{H}_0 t} A e^{-i\hat{H}_0 t}}, \hat{A}(t')] \rangle \theta(t-t')$$

$$\boxed{\chi^R(\omega) = Z^{-1} \sum_{a,b} \left(e^{-E_a/T} - e^{-E_b/T} \right) \frac{\langle a|\hat{A}|b\rangle \langle b|\hat{A}|a\rangle}{\omega + E_{ab} + i0^+}}$$

where $E_{ab} = E_a - E_b$

ensures convergence

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 $\tau = it$

$$\hat{A}(\tau) = e^{\tau H_0}\hat{A}\, e^{-\tau H_0}$$

$$0 \leq \tau, \tau' \leq \beta = 1/T \rightarrow \text{compact direction}$$

and time ordering is defined

$$T\,\hat{A}(\tau)\hat{A}(\tau') = \begin{cases} \hat{A}(\tau)\hat{A}(\tau') & \tau > \tau' \\ \hat{A}(\tau')\hat{A}(\tau) & \tau < \tau' \end{cases}$$

Since τ is periodic $\tau \simeq \tau + \beta$

$$\chi^\tau(\tau') = \sum_n e^{i\omega_n \tau}\chi^\tau(i\omega_n)$$

Matsubara frequencies $\omega_n = 2\pi n T$

We now decompose:

$$\boxed{\chi^\tau(i\omega_n) = Z^{-1}\sum_{a,b}\left(e^{-E_a/T} - e^{-E_b/T}\right) \otimes \frac{\langle a|\hat{A}|b\rangle\langle b|\hat{A}|a\rangle}{i\omega_n + E_{ab}}}$$

If we now compare spectral representations of $\chi^{R}(\omega)$ and $\chi^{\tau}(i\omega_n)$

$$\boxed{\chi^{R}(\omega) = \chi^{\tau}\left(i\omega_n \to \omega + i0^{+}\right)}$$

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

1) First compute $\chi^{\tau}(i\omega_n)$, this can be done diagrammatically or using functional integration

2) Perform analytic continuation $i\omega_n \to \omega + i0^{+}$. Given analytical expression for $\chi^{\tau}(i\omega_n)$ this is very easy. If $\chi^{\tau}(i\omega_n)$ 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)

$$j^i(\omega) = \sigma(\omega) E^i(\omega)$$

longitudinal AC conductivity

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

$$m \ddot{r}_i = -e E_i - \frac{m}{\tau} \dot{r}_i$$

friction force

introducing the velocity $\dot{r}^i = v^i$

$$-im\omega\, v_i(\omega) = -e E_i(\omega) - \frac{m}{\tau} v(\omega)$$

$$v_i(\omega) = \frac{-e E_i(\omega)}{m\left(-i\omega + \frac{1}{\tau}\right)}$$

and the current $j_i = -en v_i$ is

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

Drude AC conductivity

ballistic regime

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

$\omega \ll \tau^{-1}$ $\quad \sigma(\omega) \approx \frac{ne^2\tau}{m} \rightarrow$ 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 el-mag current j_μ to external gauge potential A_ν : $\mu, \nu = t, x, y, z$

$$\langle j_\mu(x) \rangle = \int_{t'<t} dx \; K_{\mu\nu}(x, x') A_\nu(x')$$

General properties of $K_{\mu\nu}(x, x')$:

- pure gauge can not induce current

$$0 = \int dx' \, K_{\mu\nu}(x, x') \partial^\nu f(x') = \int dx' \, K_{\mu\nu}(x,x') \overleftarrow{\partial}^\nu_{x'} f$$

- current must be conserved

$$0 = \partial_\mu j^\mu(x) = \int dx' \, \partial^\mu_x K_{\mu\nu}(x, x') \, A_\nu(x')$$

$$\vec{\partial}^\mu K_{\mu\nu} = K_{\mu\nu} \overleftarrow{\partial}^\nu = 0$$

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

First we can get the current

$$\delta S \sim \int j^\mu \partial_\mu \alpha \quad \to \text{Noether current}$$

and since $\quad A_\mu \to A_\mu + \partial_\mu \alpha$

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

the expected value $\langle j^\mu \rangle$ can be extracted from logarithm of

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

define $\quad W[A] = -\log Z[A]$

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

so by construction

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

$$= \frac{\int \mathcal{D}\phi \, \frac{\delta^2 S}{\delta A_\mu \delta A_\nu} e^{-S}}{Z} - \frac{\int \mathcal{D}\phi \, \frac{\delta S}{\delta A_\mu} \frac{\delta S}{\delta A_\nu} e^{-S}}{Z}$$

$$+ \frac{\int \mathcal{D}\phi \, \frac{\delta S}{\delta A_\mu} e^{-S} \int \mathcal{D}\phi \, \frac{\delta S}{\delta A_\nu} e^{-S}}{Z^2}$$

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

diamagnetic term

paramagnetic term

Kubo formula

As example, we sketch the calculation in Euclidean effective theory of Goldstone bosons: $A_0 = i\varphi$

$$S[\theta, A_i, \varphi] = \int dx \, \frac{n_s}{2m} \left[\frac{1}{c_s^2} (D_\tau \theta)^2 + (D_i \theta)^2 \right]$$

where $D_\tau \theta = \partial_\tau \theta - \varphi$; $D_i \theta = \partial_i \theta - A_i$

Let's compute the conductivity

$$j_i(\omega, q) = \sigma(\omega, q) \, \underset{\substack{\uparrow \\ \omega A_i(\omega, q)}}{E_i(\omega, q)}$$

$$\sigma(\omega, q) = \frac{1}{\omega} K_{ii}(\omega, q) \Big|_{i\omega \to \omega + i0}$$

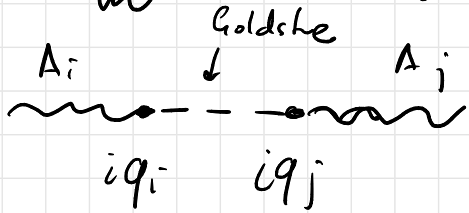
We now compute $K_{ij}(\omega, q)$ for the effective theory:

$$j^i = \frac{\delta S}{\delta A_i} = \frac{-n_s}{m} D^i \theta$$

$$\frac{\delta^2 S}{\delta A_i \delta A_j} = \frac{n_s}{m} \delta_{ij}$$

$$K_{ij}(x,x') = \frac{n_s}{m}\left(\delta_{ij} - \frac{n_s}{m}\langle \partial_i\theta \, \partial_j\theta\rangle\right)$$

Diagrammatically



In momentum space $\langle \theta_q \, \theta_{-q}\rangle = \dfrac{-m}{n\left(\frac{\omega^2}{c_s^2}+q^2\right)}$

$$K_{ij}(\omega,q) = \frac{n_s}{m}\left(\delta_{ij} - \frac{q_i q_j}{\left(\frac{\omega^2}{c_s^2}+q^2\right)}\right)$$

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

imagine we switch on a perturbation in x-dir

$q_i = (q,0)$

$$K_{xx}(\omega,q) = \frac{n_s}{m}\,\frac{\omega^2}{\omega^2+c_s^2 q^2}$$

After analytic continuation:

$$\boxed{\sigma = \frac{1}{\omega} K_{xx}\Big|_{\substack{i\omega\to\omega+i0 \\ \omega\to -i\omega}} = \frac{n_s}{m}\,\frac{i\omega}{\omega^2-c_s^2 q^2}}$$

AC conductivity $q=0$

$$\sigma(\omega) = \frac{n_s}{m}\frac{i}{\omega+i0} = \frac{in_s}{m}\left(P\frac{1}{\omega} - i\pi\delta(\omega)\right)$$

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

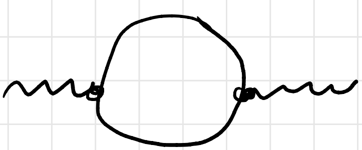
A linear response calculation of $\sigma(\omega)$ in the presence of disorder starting from the microscopic fermion theory can be found e.g. in Altland and Simons or Coleman books

Main steps:

$$K_{\mu 0}(x,x') = \underbrace{-\frac{\langle\hat{\rho}(x)\rangle}{m}\delta(x-x')\delta_{\mu 0}(1-\delta_{\mu 0})}_{\text{paramagnetic term}}$$

$$+ \langle \hat{j}^{\mu}(x)\, j^{0}(x)\rangle$$

diamagnetic term



averaging is done
1) over disorder potential
2) over state (e.g GS or thermal)

f-sum rule

Drude metal

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

Let's compute an integral

$$\int_0^\infty d\omega \, \mathrm{Re}\,\sigma(\omega) = \int_0^\infty d\omega \frac{\tau^{-1}}{\tau^{-2} + \omega^2} \times \frac{ne^2}{m}$$

$$= \frac{\pi}{2} \frac{ne^2}{2}$$

Consider now a superconductor

$$\sigma(\omega) = \frac{ne^2}{m} \frac{i}{\omega + i0}$$

$$\int_0^\infty d\omega \, \mathrm{Re}\,\sigma(\omega) = \frac{ne^2}{m} \frac{\pi}{2}$$

The integral is independent of the system. f-sum rule measures charge density

$$\boxed{\frac{2}{\pi}\int_0^\infty d\omega \, \mathrm{Re}\, \sigma(\omega) = \frac{ne^2}{m}}$$

To prove it, consider an electric pulse $E(t) = E_0 \, \delta(t)$

$$j(t=\delta) = nev(t=\delta) = \frac{ne^2 E_0}{m}$$

$$\parallel$$

$$\sigma(t=\delta) E_0 = \cancel{E_0}\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega\delta} \sigma(\omega) = \frac{ne^2}{m}\cancel{E_0}$$

now we use

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \sigma(\omega + i0) e^{-i\omega\delta} = \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \mathrm{Re}\,\sigma(\omega)$$

substituting this into the previous expression proves the f-sum rule

Different systems have the AC weight distributed differently