Linear response theory

Different ways of probing the system: (AS 7.1)

* thermodynamics
* transport
* spectroscopy.

We ~~to~~ probe the system w/ a <u>weak</u>, (additional) interaction, coupling to $\hat{X}'$:

$$H_F = F(t)\,\hat{X}'(t), \quad \text{w/ } F \text{ some 'force'}.$$

$$= \int d^d r\, F(\vec{r},t)\,\hat{X}'(\vec{r},t)$$

We measure some quantity $\hat{X}(t)$, that would give zero w/o F:

$$X(t) = \langle \hat{X}(t) \rangle = \int_{-\infty}^{t} dt' \int d^d r'\, \chi(\vec{r},\vec{r}',t,t')\, F(\vec{r}',t') + O(F^2)$$

Ex: we apply an el. static potential, that couples to electron density, and measure this density (or a current)

$$F(\vec{r},t) = \phi(\vec{r},t), \quad X'(t) = \rho(\vec{r},t)$$

$$X(t) = j(\vec{r},t)$$

Task: calculate the response function χ

(gen. susceptibility)

Gen. properties: if H_0 does not depend on time:
χ depends on $t-t'$, where $t > t'$

So, we write: $X(r,\omega) = \int d^d r' \chi(r,r',\omega) F(r',\omega) + O(F^2)$

So, if we drive at ω, and get response at some <u>other</u> frequency, we know that the response is <u>non</u> linear.

For translation inv. systems, we write

$$X(q,\omega) = \chi(q,\omega) F(q,\omega) + O(F^2).$$

We are interested in time dep. quantities, but we know how to calculate $\langle \hat{X}(\tau) \rangle$ in imaginary time. So, we need to 'Wick rotate back', and find link between real & imaginary time correlation functions.

The imaginary time correlation function is def as:

$$C^{T}_{X_1X_2}(\tau_1-\tau_2) := -\langle T_\tau \hat{X}_1(\tau_1)\hat{X}_2(\tau_2)\rangle$$
$$= -\begin{cases} \langle \hat{X}_1(\tau_1)\hat{X}_2(\tau_2)\rangle & \tau_1 \geq \tau_2 \\ \zeta_X \langle \hat{X}_2(\tau_2) X_1(\tau_1)\rangle & \tau_2 > \tau_1 \end{cases}$$

w/ $X_i = X_i(c, c^+)$ $\hookrightarrow -1$ if $\hat{X}_i$ fermionic

The real time version is: $(\tau \to it)$

$$C^{T}_{X_1X_2}(t_1-t_2) = -i\langle T_t \hat{X}_1(t_1)\hat{X}_2(t_2)\rangle,$$

(factor of i is for convenience).

But, this is not the correlator that is most relevant physically!

We want to calculate $X(t) = \langle \hat{X}^F(t)\rangle$,

where $H = H_0 + H_F$ (note H_0 can contain interactions!)

we use 'interaction picture':

$$X(t) = U_F^+(t)\,\hat{X}_I(t)\,U_F(t),$$ with

$\hat{X}_I$ the Heisenberg fields, w/o. the perturbation.

$$U_F(t) = U_F(t,-\infty) = T_t\, e^{-\frac{i}{\hbar}\int_{-\infty}^{t} dt'\, H_F(t')}$$

to lin. order in t:

$$U_F(t) = 1 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, \hat{X}'_I(t')\, F(t')$$

So, we obtain:

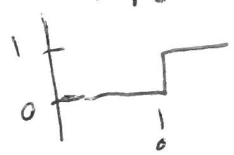
$$X(t) = \langle -\infty | U_F^{+}(t)\, X_I(t)\, U_F(t) | -\infty \rangle,$$

and we assume we switch on pert. adiabatically in the far past, so we stay in ground state.

$$X(t) = \langle 0| \left(1 + \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, X'(t')\, F(t')\right) \hat{X}_I(t) \left(1 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, X'(t')\, F(t')\right)|0\rangle$$

We assume that $\langle 0| \hat{X}_I(t) |0\rangle = 0$, and get

$$X(t) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt'\, \underbrace{\vartheta(t-t')}_{\text{stepfunction}}\, \langle 0| \hat{X}_I(t)\, X'(t') - X'(t')\, X_I(t) |0\rangle \times F(t')$$



$$= -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt'\, \vartheta(t-t')\, F(t) \langle [X_I(t), X'(t')] \rangle$$

$$:= \int dt'\, C^{+}_{XX'}(t-t')\, F(t'),$$

where $C^{+}_{XX'}(t_1-t_2) = -i\,\vartheta(t_1-t_2) \langle [\hat{X}(t_1), \hat{X}'(t_2)] \rangle$ $(\hbar = 1)$

is the <u>retarded</u> response function

(nonzero only then $t_1 > t_2$: <u>causality</u>).

We also define the advanced response function:

$$C^{-}_{XX'}(t_1 - t_2) = +i\,\theta(t_2 - t_1)\,\langle [\hat{X}(t_1), \hat{X}'(t_2)] \rangle$$

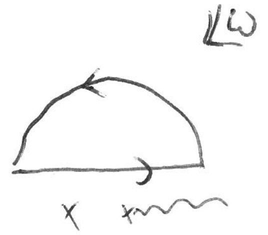
~~and then~~ Note: $C^{+}_{XX'}(t-t')$ is the susceptibility!

If we have time invariance:

$$\chi(t,t') = \chi(t-t') = \int \frac{d\omega}{2\pi}\, e^{-i\omega(t-t')}\, \chi(\omega)$$

Should be zero for $t < t'$

This is the case if all singularities of $\chi(\omega)$ are <u>below</u> the real axis!



How do we calculate the retarded real time correlator C^{+}. We have access to C^{τ}, the τ-ordered (imag. time) correlator.

Need relation between the various correlators!

We use the Lehmann representation:

assume we have a complete set of eigenstates $\{|\Psi_\alpha\rangle\}$ (Note: we hardly have access, but we use it to show the connections).

The thermal exp. values: $\mathrm{tr}(\cdots) = \sum_\alpha \langle\Psi_\alpha|\cdots|\Psi_\alpha\rangle$, and we insert $\mathbb{1} = \sum_\beta |\Psi_\beta\rangle\langle\Psi_\beta|$ in between the operators X_1 X_2:

$$C^T(t) = -i\, Z^{-1} X_{1,\alpha\beta} X_{2\beta\alpha}\, e^{it(\xi_\alpha - \xi_\beta)} \times$$

$$\times \left(\theta(t)\, e^{-\beta \xi_\alpha} + \zeta_x\, \theta(-t)\, e^{-\beta\xi_\beta} \right),$$

$\xi_\alpha = E_\alpha - \mu N_\alpha$; eigenvalue of $|\Psi_\alpha\rangle$; $X_{\alpha\beta} = \langle\Psi_\alpha|X|\Psi_\beta\rangle$

Doing the fourier transform:

$$C^T(\omega) = \int_{-\infty}^{\infty} dt\, C^T(t)\, e^{i\omega t - \eta|t|}$$

for convergence.

$$= Z^{-1} X_{1\alpha\beta} X_{2\beta\alpha} \left[\frac{e^{-\beta\xi_\alpha}}{\omega + (\xi_\alpha - \xi_\beta) + i\eta} - \zeta_x \frac{e^{-\beta\xi_\beta}}{\omega + (\xi_\alpha - \xi_\beta) - i\eta} \right]$$

The retarded and advances version differ in the $i\eta$ description:

$$C^+(\omega) = \cdots \left[\frac{1}{+i\eta} - \frac{1}{+i\eta} \right]$$

$$C^-(\omega) = \left[\frac{1}{-i\eta} - \frac{1}{-i\eta} \right]$$

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So $C^+(\omega)$ is analytic in upper half plane, so it is retarded.

One can show that $C^T(\omega)$, $C^+(\omega)$ and $C^-(\omega)$ contain the same information

[use $\lim_{\eta \to 0} \frac{1}{x \pm i\eta} = \mp i\pi\delta(x) + P.V. \frac{1}{x}$] Dirac id.

Let's look at the img. time version:

$$C^T(\tau) = -Z^{-1} X_{1\alpha\beta} X_{2\beta\alpha} e^{(\xi_\alpha - \xi_\beta)\tau} \left[\theta(\tau) e^{-\beta\xi_\alpha} - \zeta_X \theta(-\tau) e^{-\beta\xi_\beta}\right],$$

which has the property: $C^T(\tau) = \zeta_X C^T(\tau+\beta)$

(exc.), so we can use Matsubara representation:

$$C^T(i\omega_n) = \int_0^\beta d\tau \, C^T(\tau) e^{i\omega_n \tau}$$

$$= Z^{-1} \frac{X_{1\alpha\beta} X_{2\beta\alpha}}{i\omega_n + (\xi_\alpha - \xi_\beta)} \left[e^{-\beta\xi_\alpha} - \zeta_X e^{-\beta\xi_\beta}\right]$$

So, we define

$$C(z) = Z^{-1} \frac{X_{1\alpha\beta} X_{2\beta\alpha}}{z + (\xi_\alpha - \xi_\beta)} \left[e^{-\beta\xi_\alpha} - \zeta_X e^{-\beta\xi_\beta}\right],$$

which gives C^+, C^-, C^T if evaluated at $\omega^+, \omega^-, i\omega_n$

Analitic everywhere, except for the real axis.

So, if we know $C^T(i\omega_n)$ for all positive ω_n, we can analitically continue to upperhalf plane, ~~and~~ i.e. to $\omega + i0$, which gives us the wanted $C^+(\omega)$.

Ex: Greens function: $\hat{X}_1 = c_a$, $\hat{X}_2 = c_a^+$:

$$\mathcal{G}_a(\omega_n) = \frac{1}{i\omega_n - \xi_a} \rightsquigarrow \mathcal{G}_a^+(\omega) = \frac{1}{\underbrace{\omega + i0}_{=\omega^+} - \xi_a}$$

or, w/ a selfenergy:

$$\mathcal{G}_a(\omega_n) = \frac{1}{i\omega_n - \xi_a - \Sigma(i\omega_n)} \to \mathcal{G}_a^+(\omega) = \frac{1}{\omega^+ - \xi_a - \Sigma(\omega^+)}$$

Spectral function:

$$A(\omega) \equiv -2\,\mathrm{Im}\, C^+(\omega)$$

$$= 2\pi Z^{-1} X_{1\alpha\beta} X_{2\beta\alpha} \left[e^{-\beta\xi_\alpha} - \xi_\lambda e^{-\beta\xi_\beta}\right] \delta(\omega + \xi_\alpha - \xi_\beta)$$

What is the meaning.

Take $X_1 = c_a$, $X_2 = c_a^+$; $H = H_0$ (non-interacting)

$\rightsquigarrow A_a(\omega) = 2\pi\,\delta(\omega - \xi_a)$, peaked at the single particle energies. Interactions lead to broading of peaks.

The spectral function contains the same information as $C(z)$?

Write $A(\omega) = i\,(\underset{\uparrow\,\text{anal. uhp}(\omega)}{C^+(\omega)} - \underset{\uparrow\,\text{anal. lhp}(\omega)}{C^-(\omega)})$, and one ~~can~~ can show:

$$C(z) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(\omega)}{z-\omega}$$

For $\operatorname{Im}(z) > 0$: C^- cont. vanishes (close contour in lhp) no singularities

$$C^+ \text{ cont: } -\frac{1}{2\pi i} \int_{\gamma\,(\text{uhp})} d\omega \, \frac{C^+(\omega)}{z-\omega} = C(z)$$

If $\operatorname{Im}(z) < 0$, similar arguement!

So, if we know im. part of $C^+(\omega)$, i.e. $A(\omega)$, we can reconstruct $C(z)$, but we need ~~all~~ to know it for <u>all</u> frequencies!).

<u>Kramers-Kronig relation</u>: $z = \omega^+$:

$$C^+(\omega) = -\frac{1}{2\pi i} \int d\omega' \, \frac{C^+(\omega')}{\omega - \omega' + i0}$$, or w/ dirac Id:

$$C^+(\omega) = \frac{1}{\pi i} \int d\omega' \, C^+(\omega') \, PV\left(\frac{1}{\omega' - \omega}\right)$$, or

$$\operatorname{Re} C^+(\omega) = \frac{1}{\pi} \int d\omega' \, \cancel{E} \operatorname{Im}(C^+(\omega')) \, PV\left(\frac{1}{\omega' - \omega}\right)$$