LINEAR RESPONSE AND LEHMANN'S REPRESENTATION

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1. Linear Response

To investigate the properties of a system, one has to interact with it. If the interaction is weak, information about unperturbed properties may be gathered. In the linear regime, a measurement of an observable gives the deviation from the equilibrium value that is proportional to the perturbing field. The proportionality is through a response function that is a property of the unperturbed system (such as conductivity, dielectric function, magnetic susceptibility, ...).
The theory of linear response provides an expression for such functions.

Let $\hat H$ be the Hamiltonian of the system under investigation. The interaction with an external field gives a time-dependent Hamiltonian

$$\hat H(t) = \hat H + \hat V(t), \qquad \hat V(t) = 0 \text{ for } t < 0$$

The state at $t \le 0$ is the ground state $|E_0\rangle$ of H. For $t > 0$ the state is $|\Psi(t)\rangle = \hat U(t,0)|E_0\rangle = e^{-\frac{i}{\hbar}\hat H t}\hat U_I(t,0)|E_0\rangle$. An observable $\hat O$ has mean value

$$\langle\Psi(t)|\hat O|\Psi(t)\rangle = \langle E_0|\hat U_I(t,0)^\dagger \hat O_H(t)\hat U_I(t,0)|E_0\rangle$$
$$\hat U_I(t,0) = \mathsf{T}\exp\frac{1}{i\hbar}\int_0^t dt'\hat V_H(t')$$

In the linear regime we only keep terms linear in V, then:

$$\langle\Psi(t)|\hat O|\Psi(t)\rangle - \langle E_0|\hat O|E_0\rangle = \frac{1}{i\hbar}\int_0^t dt'\langle E_0|\,[\hat O_H(t),\hat V_H(t')]\,|E_0\rangle$$

The left-hand-side is the measured variation $\delta O(t)$ induced by the perturbation. In the right-hand side, we exploit $V(t) = 0$ for $t < 0$, to rewrite the result.
This is the simple general formula for linear response (Ryogo Kubo, 1957):

$$\delta O(t) = \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt'\theta(t-t')\langle E_0|\,[O_H(t),V_H(t')]\,|E_0\rangle \tag{1}$$

The theta function enforces causality: the observed effect at time t only depends on the perturbation at earlier times.
To identify a response function, we consider two important cases.

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Perturbation coupled to the density. $\hat{V}(t) = \int d\mathbf{x}\, \hat{n}(\mathbf{x})\varphi(\mathbf{x},t)$, where $\hat{n}(\mathbf{x})$ is the density of particles of the system and $\varphi(x)$ is an external field that is zero for $t<0$. The coupling to the density is appropriate to evaluating the variation of the density (we omit the specification H for the Heisenberg evolution):

$$\delta n(\mathbf{x},t) = \frac{1}{i\hbar}\int_{-\infty}^{+\infty} dt' \int d\mathbf{x}' \theta(t-t')\langle E_0|\,[\hat{n}(\mathbf{x},t),\hat{n}(\mathbf{x}',t')]\,|E_0\rangle \varphi(\mathbf{x}',t')$$

The response function is the *retarded correlator*:

$$\delta n(x) = \frac{1}{\hbar}\int d_4x' D^{\mathsf{ret}}(x,x')\varphi(x') \tag{2}$$

$$iD^{\mathsf{ret}}(x,x') = \theta(t-t')\langle E_0|\,[\hat{n}(x),\hat{n}(x')]\,|E_0\rangle \tag{3}$$

If the system is invariant for space-time translations, the correlator depends on $x-x'$, and eq.(2) is a convolution integral. In Fourier space the Fourier modes decouple and *respond independently*:

$$\boxed{\delta n(k) = \frac{1}{\hbar} D^{\mathsf{ret}}(k)\varphi(k)} \tag{4}$$

Exercise 1.1. *Show that* $\Pi^{\mathsf{T}}(k) = \Pi^{\mathsf{T}}(-k)$, $\Pi^{\mathsf{R}}(k)^* = \Pi^{\mathsf{R}}(-k)$.

Perturbation coupled to the current. For particles with charge q, the Hamiltonian H minimally coupled to a vector field is:

$$\hat{H}(t) = \hat{H} - \frac{q}{c}\int d\mathbf{x}\, \hat{\mathbf{j}}(\mathbf{x})\cdot\mathbf{A}(\mathbf{x},t) + \frac{q^2}{2mc^2}\int d\mathbf{x}\, \hat{n}(\mathbf{x})A^2(\mathbf{x},t) \tag{5}$$

with $\hat{j}_k(\mathbf{x}) = \frac{i\hbar}{2m}\sum_\sigma[(\partial_k\psi_\sigma^\dagger)(\mathbf{x})\psi_\sigma(\mathbf{x}) - \psi_\sigma^\dagger(\mathbf{x})(\partial_k\psi_\sigma^\dagger)(\mathbf{x})]$ (density current).
The charged current density is the vector operator $\hat{\mathbf{J}}(\mathbf{x},t) = q\hat{\mathbf{j}}(\mathbf{x}) - \frac{q^2}{mc}\hat{n}(\mathbf{x})\mathbf{A}(\mathbf{x},t)$. For $t<0$ there is no current. For $t>0$, in linear response it is (equal indices are summed):

$$J_j(x) = -\frac{q^2}{mc}\langle E_0|n(\mathbf{x})|E_0\rangle A_j(x) - \frac{q^2}{\hbar c}\int d_4x'\; D^{\mathsf{ret}}_{jk}(x,x')A_k(x') \tag{6}$$

$$iD^{\mathsf{ret}}_{jk}(x,x') = \theta(t-t')\langle E_0|\,[j_j(x),j_k(x')]\,|E_0\rangle \tag{7}$$

In a homogeneous system, with uniform density n:

$$J_j(k) = \left[-\frac{q^2}{mc}n\delta_{jk} - \frac{q^2}{\hbar c}D_{jk}(k)\right]A_k(k) \tag{8}$$

If the vector potential describes an electric field, $\mathbf{E}(\mathbf{k},\omega) = \frac{i\omega}{c}\mathbf{A}(\mathbf{k},\omega)$, then the induced current density is

$$J_j(k) = \sigma_{jk}(k)E_k(k), \quad \sigma_{jk}(k) = -\frac{q^2}{im\omega}n\delta_{jk} - \frac{q^2}{i\hbar\omega}D_{jk}(k)$$

σ_{jk} is the conductivity tensor. In the textbook by Mahan [4] it is evaluated in a model of independent electrons in a medium of randomly placed potential scatterers.

2. The Lehmann representation

The retarded correlators that appear in Linear Response can be evaluated from time-ordered correlators via the Lehmann representation in frequency space.
Let us consider the correlators of two observables $\hat{A}$ and $\hat{B}$ that evolve in time according to a time-independent Hamiltonian with eigenstates $\hat{H}|E_n\rangle = E_n|E_n\rangle$ ($|E_0\rangle$ is the ground state). The correlators are functions of $t-t'$.

$$iC^{\mathsf{ret}}_{AB}(t-t') = \langle E_0|[\hat{A}(t),\hat{B}(t')]|E_0\rangle\theta(t-t') \tag{9}$$

$$\begin{aligned} iC^{\mathsf{T}}_{AB}(t-t') &= \langle E_0|\mathsf{T}\delta\hat{A}(t)\delta\hat{B}(t')|E_0\rangle \\ &= \langle E_0|\mathsf{T}\hat{A}(t)\hat{B}(t')|E_0\rangle - \langle E_0|\hat{A}|E_0\rangle\langle E_0|\hat{B}|E_0\rangle \end{aligned} \tag{10}$$

The operators $\hat{A}(t)$ and $\hat{B}(t)$ commute in the T ordering.

In frequency space the correlators have the following Lehmann representations:

$$\boxed{C^{\mathsf{ret}}_{AB}(\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{C_{AB}(\omega')}{\omega-\omega'+i\eta}, \quad C^{\mathsf{T}}_{AB}(\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{C_{AB}(\omega')}{\omega-\omega'+i\eta\,\mathrm{sign}\,\omega'}} \tag{11}$$

with the *spectral function*

$$C_{AB}(\omega) = \sum_{n>0}\Big[A_{0n}B_{n0}\delta(\omega - \tfrac{E_n-E_0}{\hbar}) - B_{0,n}A_{n,0}\delta(\omega + \tfrac{E_n-E_0}{\hbar})\Big] \tag{12}$$

and matrix elements $A_{0,n} = \langle E_0|A|E_n\rangle$ etc.

Proof. Insertion of the completeness $\sum_{n\ge 0}|E_n\rangle\langle E_n|$ in the retarded correlator (9) and the action of the time-evolution on the eigenstates makes time dependence explicit:

$$iC^{\mathsf{ret}}_{AB}(t-t') = \theta(t-t')\sum_n [A_{0,n}B_{n,0}e^{-\frac{i}{\hbar}(E_n-E_0)(t-t')} - B_{0n}A_{n0}e^{\frac{i}{\hbar}(E_n-E_0)(t-t')}]$$

Note that the term $n=0$ cancels in the sum. The Fourier representation of the Heaviside function is now used:

$$\theta(t-t') = i\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\frac{e^{-i\omega(t-t')}}{\omega+i\eta}$$

After shifts of the variable ω one obtains the Fourier integral

$$C^{\mathsf{ret}}_{AB}(t-t') = \int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-i\omega(t-t')}C^{\mathsf{ret}}_{AB}(\omega)$$

$$C^{\mathsf{ret}}_{AB}(\omega) = \sum_{n>0}\left[\frac{A_{0,n}B_{n,0}}{\omega - \frac{E_n-E_0}{\hbar} + i\eta} - \frac{B_{0,n}A_{n,0}}{\omega + \frac{E_n-E_0}{\hbar} + i\eta}\right] \tag{13}$$

Similarly, insertion of the completeness in the time-ordered correlator (10) gives:

$$\begin{aligned} iC^{\mathsf{T}}_{AB}(t-t') =&\theta(t-t')\sum_{n\ge 0}A_{0,n}B_{n,0}e^{-\frac{1}{\hbar}(E_n-E_0)(t-t')} \\ &+\theta(t'-t)\sum_{n\ge 0}B_{0,n}A_{n,0}e^{\frac{1}{\hbar}(E_n-E_0)(t-t')} - A_{0,0}B_{0,0} \end{aligned}$$

The term $n=0$ in the sum cancels the term $A_{0,0}B_{0,0}$ (this is the reason for considering the time-ordered correlator of fluctuations $\delta A = A - A_{00}$. We could as well consider $[\delta A(t), \delta B(t)]$ without any change in eq.(9)).

The insertion of the Fourier integrals of the Heaviside functions, and shifts in ω give the expression

$$C^{\mathsf{T}}_{AB}(\omega) = \sum\nolimits_{n>0} \left[\frac{A_{0,n}B_{n,0}}{\omega - \frac{E_n-E_0}{\hbar} + i\eta} - \frac{B_{0,n}A_{n,0}}{\omega + \frac{E_n-E_0}{\hbar} - i\eta} \right]$$

The Lehmann expressions are obtained, with the same spectral function. □

Remark 2.1. *Since $E_n - E_0 > 0$, the two delta functions in the spectral function* (13) *are mutually exclusive.*
The poles of a retarded correlator only occur in $\mathrm{Im}\,\omega < 0$.
The poles ω_a of a time-ordered correlator have $\mathrm{Im}\,\omega_a$ *with opposite sign of* $\mathrm{Re}\,\omega_a$.

2.1. **Kramers-Krönig relations.**

$$\mathrm{Re}\, C^{\mathsf{ret}}_{AB}(\omega) = \fint_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im}\, C^{\mathsf{ret}}_{AB}(\omega')}{\omega' - \omega} \tag{14}$$

$$\mathrm{Im}\, C^{\mathsf{ret}}_{AB}(\omega) = -\fint_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Re}\, C^{\mathsf{ret}}_{AB}(\omega')}{\omega' - \omega} \tag{15}$$

Proof. The retarded correlator is analytic in $\mathrm{Im}\,\omega > 0$. For ω real consider the closed contour γ given by the segment $[-R, R]$ closed by a half-circle of radius R in the upper half-plane. The following integral is zero:

$$\oint_\gamma \frac{d\omega'}{2\pi i} \frac{C^{\mathsf{ret}}_{AB}(\omega')}{\omega' - \omega + i\eta} = 0$$

If $R\, C^{\mathsf{ret}}_{AB}(Re^{i\theta})$ vanishes for large R, we obtain:

$$0 = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \frac{C^{\mathsf{ret}}_{AB}(\omega')}{\omega' - \omega + i\eta} = \fint_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \frac{C^{\mathsf{ret}}_{AB}(\omega')}{\omega' - \omega} - \frac{1}{2} C^{\mathsf{ret}}_{AB}(\omega)$$

We used the Plemelj - Sokhotski formula

$$\frac{1}{x - y \pm i\eta} = \frac{P}{x - y} \mp i\pi\delta(x - y) \tag{16}$$

Separation of real and imaginary parts gives the results. □

2.2. **Lehmann representation with translation invariance.**
The relation beween retarded and time-ordered correlators is more explicit for local operators if $\hat{H}$ is invariant for space translations, $[H, \mathbf{P}] = 0$. The eigenstates of $\hat{H}$ and $\hat{\mathbf{P}}$ are now $|E_{n,\mathbf{k}}, \mathbf{k}\rangle$, with eigenvalues $E_n(\mathbf{k})$ and $\hbar\mathbf{k}$. We assume that the ground state has zero momentum: $\hat{\mathbf{P}}|E_0\rangle = 0$.

Consider the operators $\hat{n}(\mathbf{x})$ and $\hat{n}(\mathbf{y})$. With the operator identity $\hat{n}(\mathbf{x}) = e^{-\frac{i}{\hbar}\mathbf{x}\cdot\hat{\mathbf{P}}}\hat{n}(\mathbf{0})e^{\frac{i}{\hbar}\mathbf{x}\cdot\hat{\mathbf{P}}}$, the matrix element is

$$\langle E_0|\hat{n}(\mathbf{x})|E_{n\mathbf{k}}, \mathbf{k}\rangle = \langle E_0|\hat{n}(\mathbf{0})|E_{n\mathbf{k}}, \mathbf{k}\rangle e^{i\mathbf{k}\cdot\mathbf{x}}$$

Then, the spectral function of the density-density correlator is:

$$D(\mathbf{x} - \mathbf{y}, \omega) = \sum_{n>0,\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \Big[|\langle E_0|\hat{n}(\mathbf{0})|E_{n\mathbf{k}}, \mathbf{k}\rangle|^2 \delta(\omega - \tfrac{E_n(\mathbf{k})-E_0}{\hbar})$$
$$- |\langle E_0|\hat{n}(\mathbf{0})|E_{n-\mathbf{k}}, -\mathbf{k}\rangle|^2 \delta(\omega + \tfrac{E_n(-\mathbf{k})-E_0}{\hbar}) \Big]$$

We read the Fourier transform

$$D(\mathbf{k},\omega) = V\sum_{n>0}\Big[|\langle E_0|n(\mathbf{0})|E_{n\mathbf{k}},\mathbf{k}\rangle|^2\delta(\omega - \tfrac{E_n(\mathbf{k})-E_0}{\hbar}) - |\langle E_0|n(\mathbf{0})|E_{n-\mathbf{k}},-\mathbf{k}\rangle|^2\delta(\omega + \tfrac{E_n(-\mathbf{k})-E_0}{\hbar})\Big]$$

The notable facts are that the spectral function is real and has the same sign of ω. The correlators in momentum space have Lehmann representations

$$D^{\mathsf{ret}}(\mathbf{k},\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{D(\mathbf{k},\omega')}{\omega - \omega' + i\eta} \tag{17}$$

$$D^{\mathsf{T}}(\mathbf{k},\omega) = \int_{-\infty}^{+\infty} d\omega' \frac{D(\mathbf{k},\omega')}{\omega - \omega' + i\eta\,\mathrm{sign}\,\omega'} \tag{18}$$

The Plemelj - Sokhotski formula (16) and separation of real and imaginary parts, give the useful relations:

$$\mathrm{Re}\,D^{\mathsf{ret}}(\mathbf{k},\omega) = \mathrm{Re}\,D^{\mathsf{T}}(\mathbf{k},\omega') \tag{19}$$

$$\mathrm{Im}\,D^{\mathsf{ret}}(\mathbf{k},\omega) = \mathrm{Im}D^{\mathsf{T}}(\mathbf{k},\omega)\,\mathrm{sign}\,\omega \tag{20}$$

2.3. **The retarded polarization.** The time ordered density-density correlator is, by construction, proportional to the total polarization:

$$\boxed{D^{\mathsf{T}}(x,y) = \hbar\Pi(x,y)}$$

In analogy, one defines the retarded polarization: $\hbar\Pi^{\mathsf{ret}}(x,y) = D^{\mathsf{ret}}(x,y)$. It is:

$$\mathrm{Re}\,\Pi^{\mathsf{ret}}(\mathbf{k},\omega) = \mathrm{Re}\,\Pi(\mathbf{k},\omega), \quad \mathrm{Im}\,\Pi^{\mathsf{ret}}(\mathbf{k},\omega) = \mathrm{Im}\,\Pi(\mathbf{k},\omega)\,\mathrm{sign}\omega \tag{21}$$

Define the retarded proper polarization:

$$\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega) = \mathrm{Re}\,\Pi^{\star}(\mathbf{k},\omega) + i\mathrm{Im}\,\Pi^{\star}(\mathbf{k},\omega)\mathrm{sign}\omega$$

Exercise 2.2. *Show that*

$$\Pi^{\mathsf{ret}}(\mathbf{k},\omega) = \frac{\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega)}{1 - v(\mathbf{k})\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega)} \tag{22}$$

The denominator is the retarded generalized dielectric function $\epsilon^{\mathsf{ret}}(\mathbf{k},\omega)$.

References

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