NOTES ON 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, the system is usually weakly perturbed from equilibrium, and 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 H be the Hamiltonian of the system under investigation. The interaction with an external field gives a time-dependent Hamiltonian

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

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

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

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

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

The left-hand-side is the 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. $V(t) = \int d\mathbf{x}\, n(\mathbf{x})\varphi(\mathbf{x},t)$, where $n(\mathbf{x})$ is the density of particles of the system and $\varphi(x)$ is an assigned external field that is zero for $t<0$.
This choice of perturbation is appropriate for evaluating the variation of the density:

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

The density variation is proportional to the field through a *retarded correlator*:

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

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

If the system with Hamiltonian H is homogeneous, then the correlator depends on $x-x'$, and the linear response (2) is a convolution. In Fourier components the linear response is:

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

The Fourier modes decouple and respond independently! The function $\frac{1}{\hbar}D^{\mathsf{ret}}(k)$ is a *generalized susceptibility.*

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

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

with $j_k(\mathbf{x}) = \frac{i\hbar}{2m}\sum_\sigma[(\partial_k\psi^\dagger_\sigma)(\mathbf{x})\psi_\sigma(\mathbf{x}) - \psi^\dagger_\sigma(\mathbf{x})(\partial_k\psi^\dagger_\sigma)(\mathbf{x})]$ (density current).
The charged current density is the vector operator $\mathbf{J}(\mathbf{x},t) = q\mathbf{j}(\mathbf{x}) - \frac{q^2}{mc}n(\mathbf{x})\mathbf{A}(\mathbf{x},t)$. 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:

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

If the vector potential describes an electric field, $\mathbf{E}(k) = \frac{i\omega}{c}\mathbf{A}(k)$, 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 [4] it is evaluated in a model of independent electrons in a medium of randomly placed potential scatterers.

2. The Lehmann's representation

The retarded correlators that appear in the Linear Response theory, can be evaluated from time-ordered correlators via the Lehmann representation in frequency space.
Let us consider the correlators of two observables A and B that evolve in time according to a time-independent Hamiltonian with eigenstates $H|E_n\rangle = E_n|E_n\rangle$ ($|E_0\rangle$ is the ground state):

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

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

The operators $A(t)$ and $B(t)$ commute in the T ordering. The correlators are functions of $t-t'$.

In frequency space they 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*

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

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:

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

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 final 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 Im $\omega < 0$.
The poles of a time-ordered correlator have Im ω *with opposite sign of* Re ω.

Proposition 2.2 (Kramers-Krönig relations)**.**

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

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

Proof. The retarded correlator is analytic in 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 $R\, C^{ret}_{AB}(Re^{i\theta})$ vanishes for large R, we obtain: $0 = \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi i} \frac{C^{\mathsf{ret}}_{AB}(\omega')}{\omega' - \omega + i\eta}$. With the Plemelj - Sokhotski formula

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

we have, for real ω:

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

Separation of real and imaginary parts gives the results. □

Lehmann representation with translation invariance.
The relation beween retarded and time-ordered correlators becomes more explicit for local operators in presence of space-translation symmetry of the Hamiltonian, $[H, \mathbf{P}] = 0$. The eigenstates of H and $\mathbf{P}$ 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: $\mathbf{P}|E_0\rangle = 0$.

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

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

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

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

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:

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

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

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

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

One also defines the retarded polarization: $\hbar\Pi^{\mathsf{ret}}(x,y) = D^{\mathsf{ret}}(x,y)$.
With translation invariance:

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

If we define $\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega) = \mathrm{Re}\,\Pi^\star(\mathbf{k},\omega) + i\mathrm{Im}\,\Pi^\star(\mathbf{k},\omega)\mathrm{sign}\omega$, then it follows that:

$$\Pi^{\mathsf{ret}}(\mathbf{k},\omega) = \frac{\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega)}{1-v(\mathbf{k})\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega)} \tag{21}$$

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

Dielectric function in homogeneous electron gas. In linear response, the variation of the electron charge density (the induced charge density) in response to the perturbation caused by the electrostatic potential of an external charge density $\rho^{ext}(\mathbf{x},t)$ is:

$$-e\delta n(x) = \frac{e^2}{\hbar}\int d_4x' D^{\mathsf{ret}}(x,x')\int d_4x'' \frac{\delta(t'-t'')}{|\mathbf{x}'-\mathbf{x}''|}\rho^{ext}(x'')$$

If the unperturbed electron system is invariant for space translations, the retarded function depends on $x-x'$. In Fourier space, the induced charge is:

$$\delta\rho^{ind}(\mathbf{k},\omega) = \Pi^{\mathsf{ret}}(\mathbf{k},\omega)\frac{4\pi e^2}{\mathbf{k}^2}\rho^{ext}(\mathbf{k},\omega)$$

The Maxwell equation div$\mathbf{E} = 4\pi(\rho^{ext} + \rho^{ind})$ now is:

$$\begin{aligned} i\mathbf{k}\cdot\mathbf{E}(\mathbf{k},\omega) =& 4\pi\left[1+\Pi^{\mathsf{ret}}(\mathbf{k},\omega)\frac{4\pi e^2}{\mathbf{k}^2}\right]\rho^{ext}(\mathbf{k},\omega) \\ =& 4\pi\frac{1}{1-v(\mathbf{k})\Pi^{\star\mathsf{ret}}(\mathbf{k},\omega)}\rho^{ext}(\mathbf{k},\omega) \\ =& 4\pi\frac{1}{\epsilon^{\mathsf{ret}}(\mathbf{k},\omega)}\rho^{ext}(\mathbf{k},\omega) \end{aligned}$$

This is compared with the Maxwell equation $i\mathbf{k}\cdot\mathbf{D}(\mathbf{k},\omega) = 4\pi\rho^{ext}(\mathbf{k},\omega)$.

Simple approximate expressions for the dielectric functions [2, 4] are:

$$\epsilon_{TF}(q) = 1 + \frac{q_{TF}^2}{q^2} \qquad \left(q_{TF}^2 = \frac{6\pi e^2 n_0}{E_F}\right) \qquad \text{(Thomas-Fermi)} \tag{22}$$

$$\epsilon_{RPA}^{\mathsf{ret}}(q,\omega) = 1 - \frac{4\pi e^2}{q^2}\Pi^{(0)\mathsf{ret}}(q,\omega) \qquad \text{(Lindhard)} \tag{23}$$

References

[1] A. L. Fetter and J. D. Walecka, Quantum theory of many-particle systems, McGraw Hill (1971)

[2] N. W. Ashcroft and N. D. Mermin, Solid State Physics, Holt Saunders Int. Ed. (1976)

[3] M. Dressel and G. Grüner, Electrodynamics of Solids, Cambridge (2002).

[4] G. D. Mahan, Many-Particle Physics, Kluwer Academics 3rd Ed. (2000).