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09. Linear Response and Equilibrium Dynamics

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Abstract

Part nine of course materials for Nonequilibrium Statistical Physics (Physics 626), taught by Gerhard Müller at the University of Rhode Island. Entries listed in the table of contents, but not shown in the document, exist only in handwritten form. Documents will be updated periodically as more entries become presentable.

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9. Linear Response and Equilibrium Dynamics

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Linear response and equilibrium dynamics

- Dynamics experiments in condensed matter physics
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Many-body system perturbed by radiation field

Quantum many-body system in thermal equilibrium.

Hamiltonian: $\mathcal{H}_0$.

Density operator: $\rho_0 = Z_0^{-1} e^{-\beta \mathcal{H}_0}$ with $\beta = 1/k_B T$, $Z_0 = \text{Tr}[e^{-\beta \mathcal{H}_0}]$.

Dynamical variable: $A$ (describing some attribute of system).

Heisenberg equation of motion: \[ \frac{dA}{dt} = i\frac{\hbar}{\hbar} [\mathcal{H}_0, A]. \]

Time evolution: $A(t) = e^{i\mathcal{H}_0 t/\hbar} A e^{-i\mathcal{H}_0 t/\hbar}$ (formal solution).

Stationarity, $[\rho_0, \mathcal{H}_0] = 0$, implies time-independent expectation values:
\[
\langle A(t) \rangle_0 = \frac{1}{Z_0} \text{Tr} \left[ e^{-\beta \mathcal{H}_0} e^{i\mathcal{H}_0 t/\hbar} A e^{-i\mathcal{H}_0 t/\hbar} \right] = \frac{1}{Z_0} \text{Tr} \left[ e^{-\beta \mathcal{H}_0} A \right] = \text{const}.
\]

Time-dependent quantities do exist in thermal equilibrium!

Dynamic correlation function: $\langle A(t)A(0) \rangle_0 = \frac{1}{Z_0} \text{Tr} \left[ e^{-\beta \mathcal{H}_0} e^{i\mathcal{H}_0 t/\hbar} A e^{-i\mathcal{H}_0 t/\hbar} A \right]$

In an experiment the system is necessarily perturbed:
\[
\mathcal{H}(t) = \mathcal{H}_0 - b(t)B,
\]

where $b(t)$ is some kind of radiation field (c-number) and $B$ is the dynamical system variable (operator) to which the field couples.

Examples:

<table>
<thead>
<tr>
<th>$b(t)$</th>
<th>$B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>magnetic field</td>
<td>magnetization</td>
</tr>
<tr>
<td>electric field</td>
<td>electric polarization</td>
</tr>
<tr>
<td>sound wave</td>
<td>particle density</td>
</tr>
</tbody>
</table>
Linear response

Radiation field $b(t)$ perturbs equilibrium state of the system $\mathcal{H}_0$ via coupling to dynamical variable $B$.

System response to perturbation measured as expectation value of dynamical variable $A$.

**Linear** response to weak perturbations is predominant under most circumstances (away from criticality).

**Response function** $\tilde{\chi}_{AB}(t)$ (definition):

$$\langle A(t) \rangle - \langle A \rangle_0 = \int_{-\infty}^{\infty} dt' \tilde{\chi}_{AB}(t-t')b(t').$$

- Linearity: $\tilde{\chi}_{AB}(t)$ is independent of $b(t)$.
- Hermiticity: $\tilde{\chi}_{AB}(t)$ is a real function.
- Causality: $\tilde{\chi}_{AB}(t) = 0$ for $t < 0$.
- Smoothness: $|\tilde{\chi}_{AB}(t)| < \infty$.
- Analyticity: $\tilde{\chi}_{AB}(t) \to 0$ for $t \to \infty$.

**Generalized susceptibility** (via Fourier transform):

$$\chi_{AB}(\zeta) = \int_{-\infty}^{+\infty} dt e^{i\zeta t} \tilde{\chi}_{AB}(t) \quad \text{(analytic for } \Im\{\zeta\} > 0).$$

Complex function of real frequency:

$$\chi_{AB}(\omega) = \lim_{\epsilon \to 0} \chi_{AB}(\omega + i\epsilon) = \chi'_{AB}(\omega) + i\chi''_{AB}(\omega).$$

Linear response in frequency domain (no mixing of frequencies):

$$\alpha(\omega) = \chi_{AB}(\omega)\beta(\omega),$$

where

$$\tilde{\chi}_{AB}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi_{AB}(\omega), \quad b(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \beta(\omega),$$

$$\langle A(t) \rangle - \langle A \rangle_0 = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t}\alpha(\omega).$$
Kubo formula for response function \([\text{nln27}]\)

Interaction representation for time evolution of \(\mathcal{H}(t) = \mathcal{H}_0 - b(t)B\):

\[
\frac{dA}{dt} = \frac{i}{\hbar} [\mathcal{H}_0, A] \quad \Rightarrow \quad A(t) = e^{i\mathcal{H}_0 t/\hbar} A e^{-i\mathcal{H}_0 t/\hbar},
\]

\[
\frac{dB}{dt} = \frac{i}{\hbar} [\mathcal{H}_0, B] \quad \Rightarrow \quad B(t) = e^{i\mathcal{H}_0 t/\hbar} B e^{-i\mathcal{H}_0 t/\hbar},
\]

\[
\frac{d\rho}{dt} = -\frac{i}{\hbar} [-b(t)B, \rho] \quad \Rightarrow \quad \rho(t) = \rho_0 + \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') [B(t'), \rho(t')].
\]

Set \(\rho(t) = \rho_0 + \rho_1(t)\) with \(\rho_0 = Z_0^{-1}e^{-\beta\mathcal{H}_0}\).

Full response: \(\langle A(t) \rangle - \langle A \rangle_0 = \text{Tr}\{\rho_1(t)A(t)\}\)

Leading correction to \(\rho_0\): \(\rho_1(t) \simeq \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') [B(t'), \rho_0]\)

Linear response:

\[
\langle A(t) \rangle - \langle A \rangle_0 = \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') \text{Tr}\{[B(t'), \rho_0]A(t)\}
\]

\[
= \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') \text{Tr}\{\rho_0[A(t), B(t')]\}
\]

\[
= \frac{i}{\hbar} \int_{-\infty}^t dt' b(t') \langle[A(t), B(t')]\rangle_0.
\]

Compare with definition of response function in \([\text{nln26}]\).

Kubo formula:

\[
\tilde{\chi}_{AB}(t - t') = \frac{i}{\hbar} \theta(t - t') \langle[A(t), B(t')]\rangle_0.
\]

- Causality requirement is ensured by step function \(\theta(t - t')\).
- Hermitian \(A, B\) imply Hermitian \(i[A, B]\). Hence \(\tilde{\chi}(t)\) is real.
- Linear response depends only on equilibrium quantities.
- Response function only depends on time difference \(t - t'\).

The Kubo formula establishes a general link between

- the dynamical properties of a many-body system at equilibrium,
- the dynamical response of that system to experimental probes.
Symmetry properties

Response function for Hermitian $A$ is real and vanishes for $t < 0$:

$$\tilde{\chi}_{AA}(t) = \frac{\hbar}{i} \theta(t) \langle [A(t), A] \rangle = \tilde{\chi}'_{AA}(t) + i \tilde{\chi}''_{AA}(t).$$

Reactive part is real and symmetric:

$$\tilde{\chi}'_{AA}(t) = \frac{1}{2} [\tilde{\chi}_{AA}(t) + \tilde{\chi}_{AA}(-t)] = \frac{\hbar}{2i} \text{sgn}(t) \langle [A(t), A] \rangle.$$

Dissipative part is imaginary and antisymmetric:

$$\tilde{\chi}''_{AA}(t) = \frac{1}{2} i [\tilde{\chi}_{AA}(t) - \tilde{\chi}_{AA}(-t)] = \frac{1}{2} \hbar \langle [A(t), A] \rangle.$$

Response function is determined by its reactive or dissipative part alone:

$$\tilde{\chi}_{AA}(t) = 2 \theta(t) \tilde{\chi}'_{AA}(t) = 2 i \theta(t) \tilde{\chi}''_{AA}(t).$$

Generalized susceptibility is complex:

$$\chi_{AA}(\omega) = \chi'_{AA}(\omega) + i \chi''_{AA}(\omega).$$

Real part is symmetric:

$$\chi'_{AA}(\omega) = \frac{1}{2} [\chi_{AA}(\omega) + \chi_{AA}(-\omega)] = \chi'_{AA}(-\omega).$$

Imaginary part is antisymmetric:

$$\chi''_{AA}(\omega) = \frac{1}{2i} [\chi_{AA}(\omega) - \chi_{AA}(-\omega)] = - \chi''_{AA}(-\omega).$$
Kramers-Kronig dispersion relations

Use analyticity of $\chi_{AA}(\zeta)$ for $\Im\{\zeta\} > 0$.

Cauchy integral: $\chi_{AA}(\zeta) = \frac{1}{2\pi i} \int_{C} d\zeta' \frac{\chi_{AA}(\zeta')}{\zeta' - \zeta}$.

Integral converges for $\zeta' = \omega' + i\epsilon'$, $\epsilon' \to 0$.
Integral along semi-circle vanishes for $R \to \infty$:
Sum rule implies $\chi_{AA}(\zeta) \lesssim |\zeta|^{-1}$ for $|\zeta| \to \infty$.

$$\Rightarrow \chi_{AA}(\zeta) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega' \frac{\chi_{AA}(\omega')}{\omega' - \zeta}.$$ 

Set $\zeta = \omega + i\epsilon$ and use $\lim_{\epsilon \to 0} \frac{1}{\omega' - \omega \mp i\epsilon} = P \frac{1}{\omega' - \omega} \pm i\pi \delta(\omega' - \omega)$.

$$\chi_{AA}(\omega) = \lim_{\epsilon \to 0} \chi_{AA}(\omega + i\epsilon) = \lim_{\epsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\omega' \frac{\chi_{AA}(\omega')}{\omega' - \omega - i\epsilon}$$
$$= \frac{1}{2\pi i} P \int_{-\infty}^{+\infty} d\omega' \frac{\chi_{AA}(\omega')}{\omega' - \omega} + \frac{1}{2} \int_{-\infty}^{+\infty} d\omega' \chi_{AA}(\omega') \delta(\omega' - \omega).$$

$$\Rightarrow \chi_{AA}(\omega) = \chi'_{AA}(\omega) + i\chi''_{AA}(\omega) = \frac{1}{\pi i} P \int_{-\infty}^{+\infty} d\omega' \frac{\chi_{AA}(\omega')}{\omega' - \omega}.$$ 

Consider real and imaginary parts of this relation separately:

$$\chi'_{AA}(\omega) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} d\omega' \frac{\chi''_{AA}(\omega')}{\omega' - \omega}, \quad \chi''_{AA}(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} d\omega' \frac{\chi'_{AA}(\omega')}{\omega' - \omega}.$$ 

The Kramers-Kronig relations are a consequence of the causality property of the response function.
Causality property of response function.

The Kramers-Kronig dispersion relations

\[
\chi'_{AA}(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega' \frac{\chi''_{AA}(\omega')}{\omega' - \omega}, \quad \chi''_{AA}(\omega) = -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega' \frac{\chi'_{AA}(\omega')}{\omega' - \omega}
\]

between the reactive part \(\chi'_{AA}(\omega)\) and the dissipative part \(\chi''_{AA}(\omega)\) of the generalized susceptibility \(\chi_{AA}(\omega)\) are a direct consequence of the causality property of the response function \(\tilde{\chi}_{AA}(t)\). Show that \(\chi_{AA}(\zeta)\) for \(\Im(\zeta) > 0\) can be expressed in terms of \(\chi''_{AA}(\omega)\) as follows:

\[
\chi_{AA}(\zeta) = \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \frac{\chi''_{AA}(\omega)}{\omega - \zeta}.
\]

Solution:
Energy transfer

Hamiltonian of system and interaction with radiation field:
\[ \mathcal{H}(t) = \mathcal{H}_0 + \mathcal{H}_1(t) = \mathcal{H}_0 - a(t)A. \]

Interaction between system and radiation field involves energy transfer.

Rate at which average energy of system changes:
\[ \frac{d}{dt} \langle \mathcal{H}_0 \rangle = \frac{1}{i\hbar} \langle [\mathcal{H}_0, \mathcal{H}(t)] \rangle = -\frac{1}{i\hbar} a(t) \langle [\mathcal{H}_0, A(t)] \rangle. \]

Calculate linear response \( \langle [\mathcal{H}_0, A(t)] \rangle - \langle [\mathcal{H}_0, A] \rangle_0 \).

Application of Kubo formula [nlh27]:
\[ \langle [\mathcal{H}_0, A(t)] \rangle = \frac{i}{\hbar} \int_{-\infty}^{t} dt' a(t') \langle [\mathcal{H}_0, A(t)] \rangle_0. \]

\[ \Rightarrow \frac{d}{dt} \langle \mathcal{H}_0 \rangle = -\frac{1}{\hbar^2} a(t) \int_{-\infty}^{t} dt' a(t') \frac{-i\hbar dA/dt}{\hbar} \langle [\mathcal{H}_0, A(t)] \rangle_0 \]
\[ = \frac{i}{\hbar} a(t) \int_{-\infty}^{t} dt' a(t') \frac{\partial}{\partial t} \langle [A(t), A(t')] \rangle_0 \]
\[ = \int_{-\infty}^{+\infty} dt' a(t) a(t') \frac{\partial}{\partial t} \tilde{\chi}_{AA}(t - t') \]
with response function
\[ \tilde{\chi}_{AA}(t - t') = \frac{i}{\hbar} \theta(t - t') \langle [A(t), A(t')] \rangle_0. \]

The time-averaged energy transfer depends only on the absorptive part, \( \chi''_{AA}(\omega) \), of the generalized susceptibility as demonstrated in [nex64] for a monochromatic perturbation.

---

1 We have \( \langle [\mathcal{H}_0, A] \rangle_0 = \text{Tr} \{ e^{-\beta \mathcal{H}_0} \mathcal{H}_0 A - e^{-\beta \mathcal{H}_0} A \mathcal{H}_0 \} / Z_0 = 0 \) in thermal equilibrium.
Reactive and absorptive parts of linear response.

In the framework of linear response theory for $H = H_0 - a(t)A$, the rate of energy transfer between the system and the radiation field is

$$\frac{d}{dt} \langle H_0 \rangle = \int_{-\infty}^{\infty} dt' a(t) a(t') \frac{\partial}{\partial t} \tilde{\chi}_{AA}(t - t'),$$

where $\tilde{\chi}_{AA}(t - t') = \langle i/\hbar \Theta(t - t') [A(t), A(t')] \rangle_0$ is the Kubo formula for the response function.

(a) Evaluate this expression for a monochromatic perturbation, $a(t) = \frac{1}{2} \alpha_m (e^{i\omega_0 t} + e^{-i\omega_0 t})$, and express it in terms of the reactive part, $\chi'_{AA}(\omega)$, and the absorptive (dissipative) part, $\chi''_{AA}(\omega)$, of the generalized susceptibility $\chi_{AA}(\omega)$.

(b) Show that the time-averaged energy transfer depends only on the absorptive part of $\chi_{AA}(\omega)$.

Solution:
Three dynamical quantities in time domain:

- $\tilde{\chi}_{AA}'(t) \doteq \frac{1}{2\hbar} \langle [A(t),A]_- \rangle$ response function (dissipative part),
- $\tilde{\Phi}_{AA}(t) \doteq \frac{1}{2} \langle [A(t),A]_+ \rangle - \langle A \rangle^2$ fluctuation function,
- $\tilde{S}_{AA}(t) \doteq \langle A(t)A \rangle - \langle A \rangle^2$ correlation function.

Relations:

$$\tilde{\chi}_{AA}'(t) = \frac{1}{2\hbar} \left[ \tilde{S}_{AA}(t) - \tilde{S}_{AA}(-t) \right], \quad \tilde{\Phi}_{AA}(t) = \frac{1}{2} \left[ \tilde{S}_{AA}(t) + \tilde{S}_{AA}(-t) \right].$$

Transformation properties under time reversal (for real $t$):

- $\tilde{\chi}_{AA}'(-t) = -\tilde{\chi}_{AA}'(t) = [\tilde{\chi}_{AA}'(t)]^*$ imaginary and antisymmetric,
- $\tilde{\Phi}_{AA}(-t) = \tilde{\Phi}_{AA}(t) = [\tilde{\Phi}_{AA}(t)]^*$ real and symmetric,
- $\tilde{S}_{AA}(-t) = \tilde{S}_{AA}(t - i\hbar \beta) = [\tilde{S}_{AA}(t)]^*$ complex.\(^2\)

To make the last symmetry relation more transparent we write

$$\langle A(-t)A \rangle = \text{Tr} \left[ e^{-\beta H_0} e^{-iH_0 t/\hbar} A e^{iH_0 t/\hbar} A \right] = \text{Tr} \left[ e^{-\beta H_0} e^{iH_0 (t-i\hbar \beta)/\hbar} A e^{-iH_0 (t-i\hbar \beta)/\hbar} A \right] = \langle A(t-i\beta \hbar)A \rangle.$$

The imaginary part of the correlation function vanishes if

- if $\beta = 0$ i.e. at infinite temperature,
- if $\hbar = 0$ i.e. for classical systems.

\(^1\)using $[\cdot]_-$ for commutators and $[\cdot]_+$ for anti-commutators.

\(^2\)with symmetric real part and antisymmetric imaginary part.
Three dynamical quantities in frequency domain:

\[ \chi''_{AA}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \tilde{\chi}''_{AA}(t) \quad \text{dissipation function,} \]

\[ \Phi_{AA}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \tilde{\Phi}_{AA}(t) \quad \text{spectral density,} \]

\[ S_{AA}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \tilde{S}_{AA}(t) \quad \text{structure function.} \]

Symmetry properties:

- \( \chi''_{AA}(-\omega) = -\chi''_{AA}(-\omega) \) real and antisymmetric,
- \( \Phi_{AA}(-\omega) = \Phi_{AA}(\omega) \) real and symmetric,
- \( S_{AA}(-\omega) = e^{-\beta \hbar \omega} S_{AA}(\omega) \) real and satisfying detailed balance.

Relations:

\[ \chi''_{AA}(\omega) = \frac{1}{2\hbar} \left( 1 - e^{-\beta \hbar \omega} \right) S_{AA}(\omega), \quad \Phi_{AA}(\omega) = \frac{1}{2} \left( 1 + e^{-\beta \hbar \omega} \right) S_{AA}(\omega). \]

Fluctuation-dissipation relation (general quantum version):

\[ \Phi_{AA}(\omega) = \hbar \coth \left( \frac{1}{2} \beta \hbar \omega \right) \chi''_{AA}(\omega). \]

Dissipation effects from an interaction with a weak external force as encoded in \( \chi''_{AA}(\omega) \) are determined by natural fluctuations existing in thermal equilibrium as encoded in \( \Phi_{AA}(\omega) \).

Classical limit (no zero-point fluctuations):

\[ \Phi_{AA}(\omega)_{cl} \xrightarrow{\hbar \to 0} \frac{2k_B T}{\omega} \chi''_{AA}(\omega). \]

Classical fluctuations of any frequency related to static susceptibility:

\[ \langle (A - \langle A \rangle)^2 \rangle = \tilde{\phi}_{AA}(t = 0) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \Phi_{AA}(\omega) = k_B T \int_{-\infty}^{+\infty} \frac{d\omega}{\pi} \omega^{-1} \chi''_{AA}(\omega) = \lim_{\omega \to 0} \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{\chi''_{AA}(\omega)}{\omega - \omega'} = \chi'_{AA}(\omega' = 0) = \chi_{AA}(\omega' = 0) = \chi_{AA}. \]
Spectral representation of dynamical quantities.

Consider a quantum Hamiltonian system with known eigenvalues and eigenvectors: $H|n\rangle = E_n|n\rangle$, $n = 0, 1, \ldots$ in thermal equilibrium at temperature $T$. Express (a) the structure function $S_{AA}(\omega)$, (b) the spectral density $\Phi_{AA}(\omega)$, (c) the dissipation function $\chi''_{AA}(\omega)$, and (d) the generalized susceptibility $\chi_{AA}(\omega + i\epsilon)$ in terms of $\beta = 1/k_B T$, $E_n$, and the matrix elements $\langle n|A|m\rangle$ under the assumption that $\langle A \rangle \equiv Z^{-1}\text{Tr}[e^{-\beta H} A] = 0$.

Solution:
Linear response of classical relaxator.

The classical relaxator is defined by the equation of motion

\[ \dot{x} + \frac{1}{\tau_0} x = a(t), \]

where \( \tau_0 \) is the relaxation time and \( a(t) \) a weak periodic perturbation. The (linear) response function is defined by the relation

\[ x(t) = \int_{-\infty}^{\infty} dt' \tilde{\chi}_{xx}(t - t') a(t'). \]

(a) Calculate the generalized susceptibility \( \chi_{xx}(\omega) \) as well as its reactive part \( \chi'_{xx}(\omega) \) and its dissipative part \( \chi''_{xx}(\omega) \). (b) Use the (classical) fluctuation-dissipation theorem to infer the spectral density \( \Phi_{xx}(\omega) \) from the dissipation function \( \chi''_{xx}(\omega) \). (c) Plot the functions \( \chi'_{xx}(\omega) \), \( \chi''_{xx}(\omega) \), and \( \Phi_{xx}(\omega) \) versus \( \omega \) for \( \tau_0 = 1 \).

Solution:
Linear response of classical oscillator.

The classical oscillator is defined by the equation of motion

\[ m \ddot{x} + \gamma \dot{x} + m\omega_0^2 x = a(t), \]

where \( \gamma \) is the attenuation coefficient, \( m\omega_0^2 \) the spring constant, and \( a(t) \) a weak periodic perturbation. The (linear) response function is defined by the relation

\[ x(t) = \int_{-\infty}^{\infty} dt' \tilde{\chi}_{xx}(t - t') a(t'). \]

(a) Calculate the generalized susceptibility \( \chi_{xx}(\omega) \) as well as its reactive part \( \chi'_{xx}(\omega) \) and its dissipative part \( \chi''_{xx}(\omega) \). (b) Use the (classical) fluctuation-dissipation theorem to infer the spectral density \( \Phi_{xx}(\omega) \) from the dissipation function \( \chi''_{xx}(\omega) \). (c) Plot the functions \( \chi'_{xx}(\omega), \chi''_{xx}(\omega), \) and \( \Phi_{xx}(\omega) \) versus \( \omega \) for \( m = \gamma = \omega_0 = 1 \).

Solution: