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International Centre for Theoretical Physics



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**School and Workshop on Highly Frustrated Magnets and Strongly
Correlated Systems: From Non-Perturbative Approaches to
Experiments**

30 July - 17 August, 2007

**Linear Response Theory and
Dynamical Correlations**

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Linear Response Theory and Dynamical Correlations

Wolfram Brenig



<http://www.fkf.mpg.de/conf/hfm2008/reg/>

Braunschweig 2008

HFM

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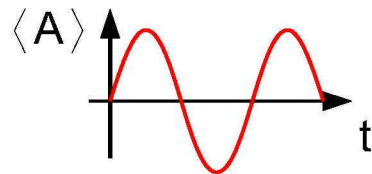
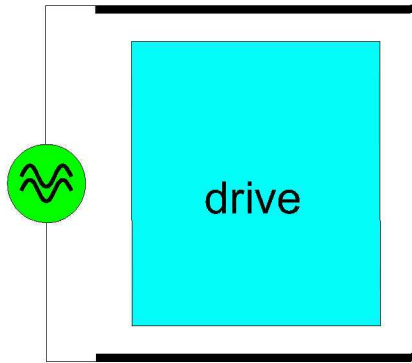
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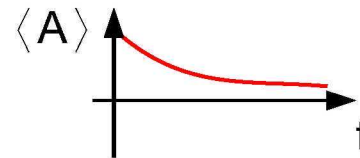
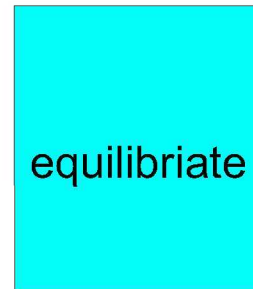
Highly Frustrated Magnetism

Three Types of Response (Functions)



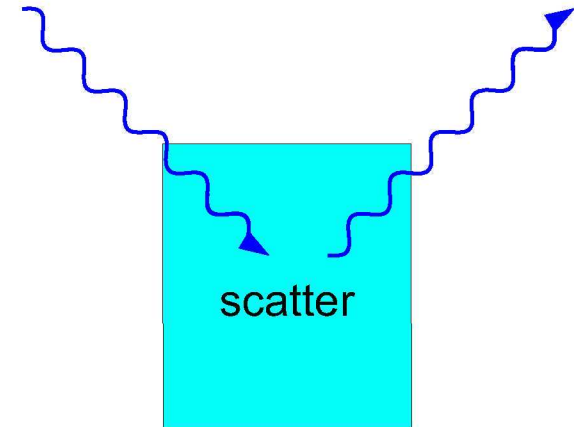
dynamical susceptibility

$$\chi(z)$$



relaxation function

$$\Phi(z)$$

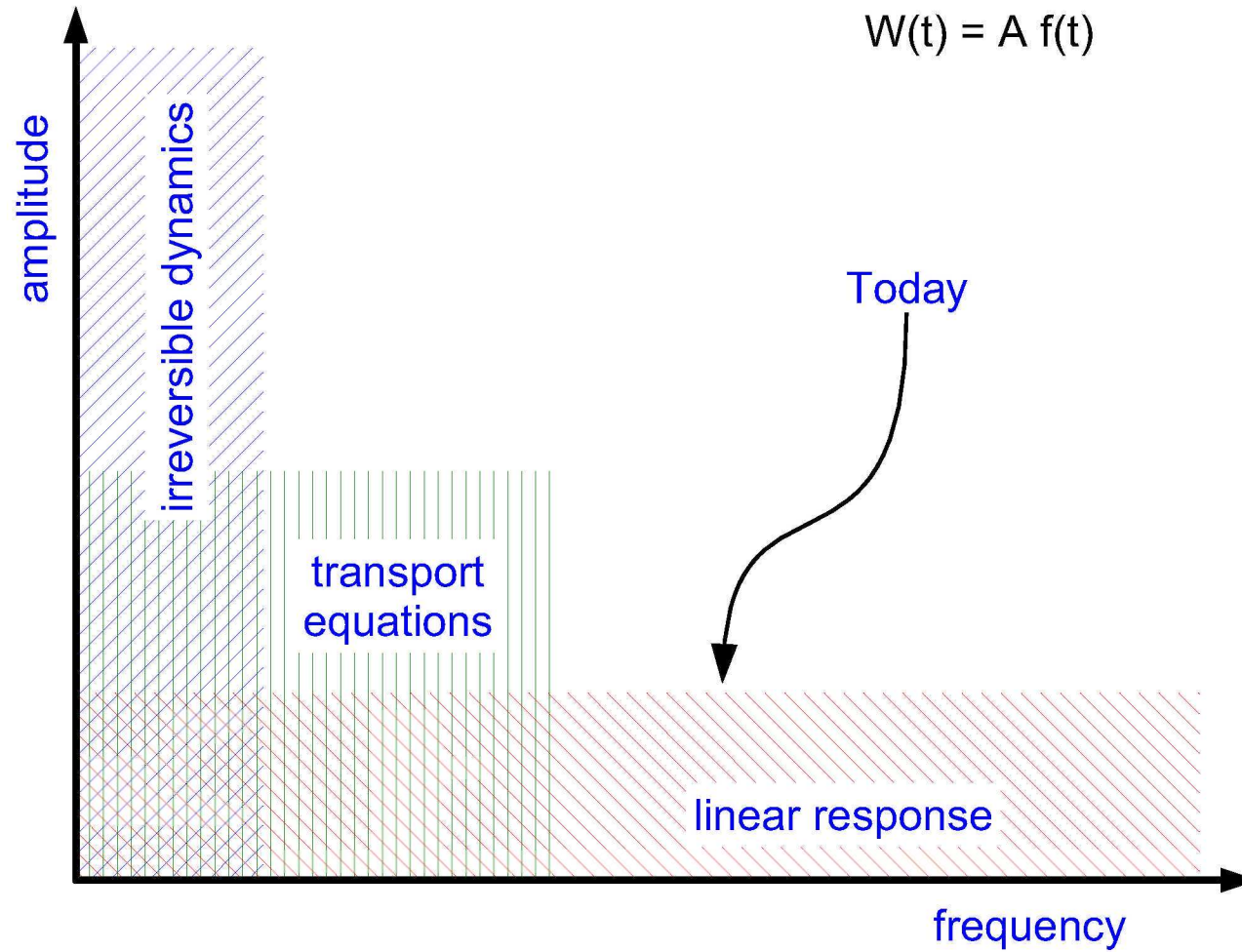


$$|i\rangle \rightarrow |f\rangle$$

dynamical correlation function

$$S(z)$$

Regimes of Dynamic Processes



Syllabus

- $\chi(z)$
 - von Neumann's Equation
 - Dynamical Susceptibility
 - Spectral Functions
 - Symmetries
 - Mori Product
 - Liouville Operator
- $\Phi(z)$
 - Relaxation Function
 - Sum Rules and Moments
- $S(z)$
 - Dynamical Correlation Function
 - Dissipation and Passivity
 - Fluctuation-Dissipation Theorem
 - Projection Technique

Literature:

D. Forster, "Hydrodynamic Fluctuations, Broken Symmetry and Correlation Functions", Addison-Wesley, 1990

E. Fick, G. Sauermaun, "The quantum statistics of dynamic processes", Springer, 1990

Dynamics of the Statistical Operator: von Neumann's Equation*

- External perturbation

$$\tilde{H} = H + W(t)$$

- von Neumann's EQM for statistical operator

$$\dot{\rho}_S(t) = -i[\tilde{H}, \rho_S(t)]$$

* Schrödinger

$$A_H(t) = e^{i\tilde{H}t} A(t) e^{-i\tilde{H}t}$$

$$\dot{\rho}_H(t) = \rho_S(0)$$

* Heisenberg

$$A_D(t) = e^{iHt} A(t) e^{-iHt}$$

$$\dot{\rho}_D(t) = -i[W_D(t), \rho_D(t)]$$

* Dirac

- Switching „on“ adiabatically from $-\infty$

$$W(t \rightarrow -\infty) = 0 \quad \text{„off“}$$

$$\Rightarrow [\rho_S(-\infty), H] = 0 \quad \text{equilib.}$$

$$\Rightarrow \rho_D(-\infty) = \rho_S(-\infty) \equiv \rho = \frac{1}{Z} e^{-\beta H}$$

- Linear regime $\|W\| \ll \|H\|$

$$\rho_D(t) = \rho - i \int_{-\infty}^t [W_D(t'), \rho] dt'$$

~~$$+ O(W^2)$$~~

! $\hbar = k_B = 1$

Linear Response: Dynamical Susceptibility

External perturbation

coordinates
forces

$$W(t) = - \sum_{\nu} A_{\nu} f_{\nu}(t)$$

coordinates,
momenta, axes,
various ops., ...

Linear response of A_{μ}^{+} to force $f_{\nu}(t)$

$$\delta \langle A_{\mu}^{+}(t) \rangle = \text{Tr} \left\{ A_{\mu D}^{+}(t) (\rho_D(t) - \rho_D(-\infty)) \right\}$$

$$\delta \langle A_{\mu}^{+}(t) \rangle = -i \int_{-\infty}^t \text{Tr} \{ A_{\mu D}^{+}(t) [W_D(t'), \rho] \} dt'$$

$$\delta \langle A_{\mu}^{+}(t) \rangle = i \sum_{\nu} \int_{-\infty}^t \langle [A_{\mu D}^{+}(t), A_{\nu D}(t')] \rangle_{\rho} f_{\nu}(t') dt'$$

'forget' D 'forget' ρ

Dynamical susceptibility

$$\delta \langle A_{\mu}^{+}(t) \rangle = \sum_{\nu} \int_{-\infty}^{\infty} \chi_{\mu\nu}(t, t') f_{\nu}(t') dt'$$

$$\chi_{\mu\nu}(t, t') = \chi_{\mu\nu}(t - t', 0) \equiv \chi_{\mu\nu}(t - t')$$

$$\chi_{\mu\nu}(t, t') = i\Theta(t - t') \langle [A_{\mu}^{+}(t), A_{\nu}(t')] \rangle = i\Theta(t - t') \chi''_{\mu\nu}(t, t')$$

①

Example:

$$H \approx \underbrace{\omega_0 b^\dagger b}_H + \underbrace{(b^\dagger + b) f(t)}_{W(t)} ; [b, b^\dagger] = 1 \text{ Bosons ; } \hbar = 1$$

$b^\dagger + b \equiv r, r^\dagger = r$

$$b(t) = e^{-i\omega_0 t} b$$

$$b^\dagger(t) = e^{i\omega_0 t} b^\dagger$$

$$\begin{aligned} \chi_{rr}(t) &= i\Theta(t) \langle [e^{-i\omega_0 t} b + e^{i\omega_0 t} b^\dagger, b + b^\dagger] \rangle \\ &= i\Theta(t) (\langle [b, b^\dagger] \rangle e^{-i\omega_0 t} + \langle [b^\dagger, b] \rangle e^{i\omega_0 t}) \\ &= i\Theta(t) (e^{-i\omega_0 t} - e^{i\omega_0 t}) \end{aligned}$$

No fact. of T !

Spectral Functions

• Spectral function χ''

$$\chi(t) := 2i\Theta(t)\chi''(t)$$

• Laplace trafo

$$\int_{-\infty}^{\infty} \frac{\chi''(\omega)}{\omega - z} \frac{d\omega}{\pi} =$$

$$\int_{-\infty}^{\infty} dt \chi''(t) \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{e^{i\omega t}}{\omega - z} = \int_0^{\infty} dt 2i\chi''(t)e^{izt}$$

$\Im z > 0$

$$= \chi(z)$$

• Retarded / Advanced

$$\chi^{R/A}(u) = \chi(u \pm i0^+) =$$

$$P \int_{-\infty}^{\infty} \frac{\chi''(\omega)}{\omega - u} \frac{d\omega}{\pi} \pm i\chi''(u) = \chi'(u) \pm i\chi''(u)$$

• Fouriertrafo of linear response

$$\delta \langle A_{\mu}^+(\omega) \rangle = \sum_{\nu} \chi_{\mu\nu}^R(\omega) f_{\nu}(\omega)$$

• Adiabatic susceptibility

$$f_{\nu}(t) = \Theta(-t)e^{0^+t} f_{\nu}$$

$$\delta \langle A_{\mu}^+(t=0) \rangle = \sum_{\nu} \int_0^{\infty} \chi_{\mu\nu}(t') e^{-0^+t'} dt' f_{\nu}$$

$$= \sum_{\nu} \chi_{\mu\nu}^R(\omega=0) f_{\nu}$$

↑
adiabatic or
isolated χ
 \neq
isothermal χ



Example

$$x_{rr}(t) = i \Theta(t) \underbrace{(e^{-i\omega_0 t} - e^{+i\omega_0 t})}$$

$$\Rightarrow x_{rr}''(t) = \frac{1}{2} \cdot \downarrow$$

$$\Rightarrow x_{rr}''(\omega) = \frac{1}{2} \int dt e^{i\omega t} (\downarrow)$$

$$= \pi [\delta(\omega - \omega_0) - \delta(\omega + \omega_0)]$$

Spectrum

$$\Rightarrow x_{rr}^{R/H}(\omega) = \int d\omega' \frac{[\delta(\omega' - \omega_0) - \delta(\omega' + \omega_0)]}{\omega' - \omega \mp i0^+}$$

$$= \frac{2\omega_0}{\omega_0^2 - (\omega \pm i0^+)^2}$$

adiabatic x_{iso}



$$x_{iso} = \frac{2}{\omega_0}$$

Symmetries

• shorthand $A_\mu^+ = A_{\bar{\mu}}$

• complex conjugation:

$$\chi''_{\mu\nu}(\omega)^* = -\chi''_{\bar{\mu}\bar{\nu}}(-\omega)$$

• commutator:

$$\chi''_{\mu\nu}(\omega) = -\chi''_{\bar{\nu}\bar{\mu}}(-\omega)$$

if: $A_\mu = A_\nu = A^+ = A$

$\Rightarrow \chi$ real & odd in ω

• parity under t-reversal

$$\pi A(t) \pi^{-1} = P^t A(-t); \quad P^t = \pm 1$$

$$\chi''_{\mu\nu}(\omega) = -P_\mu^t P_\nu^t \chi''_{\bar{\mu}\bar{\nu}}(-\omega)$$

check complex conjugation

$$\chi''_{\mu\nu}(\omega)^* =$$

$$\left(\int_{-\infty}^{\infty} dt e^{i\omega t} \frac{1}{2} \langle [A_\mu^+(t), A_\nu] \rangle \right)^* =$$

$$\int_{-\infty}^{\infty} dt e^{-i\omega t} \frac{1}{2} \langle [A_\nu^+, A_\mu(t)] \rangle =$$

$$- \int_{-\infty}^{\infty} dt e^{-i\omega t} \frac{1}{2} \langle [A_\mu^{++}(t), A_\nu^+] \rangle =$$

$$-\chi''_{\bar{\mu}\bar{\nu}}(-\omega)$$



Example

$$\chi''_{\uparrow\uparrow}(\omega) = \pi [\delta(\omega - \omega_0) - \delta(\omega + \omega_0)]$$

commutator:

$$-\chi''_{\uparrow\uparrow}(-\omega) = -\chi''_{\uparrow\uparrow}(-\omega) = \chi''_{\uparrow\uparrow}(\omega)$$

\uparrow
 $\uparrow = \uparrow = \uparrow$

complex conjugation

$$\chi''_{\uparrow\uparrow}(\omega)^* = \chi''_{\uparrow\uparrow}(\omega) = -\chi''_{\uparrow\uparrow}(-\omega)$$

t-reversal : $\pi + \pi^{-1} = +1 \uparrow$

$$\begin{aligned} \chi''_{\uparrow\uparrow}(\omega) &= -(+1)(+1) \chi''_{\uparrow\uparrow}(-\omega) \\ &= -\chi''_{\uparrow\uparrow}(-\omega) \end{aligned}$$

2a

What about:

$\chi_{\text{px}}^{\text{iso}}$
 \uparrow \sum space momentum

$$\begin{aligned} \chi''_{\text{px}}(\omega) &= -(-i)(+i) \chi''_{\text{px}}(-\omega) \\ &= \chi''_{\text{px}}(-\omega) \end{aligned}$$

$$\begin{aligned} \chi_{\text{px}}^{\text{iso}} &= \int \frac{d\omega}{\omega} \frac{\chi''_{\text{px}}(\omega)}{\omega} \\ &= 0 \end{aligned}$$

\hookrightarrow B.t.w.: what about

$\chi_{\text{PM}}^{\text{iso}}$ magnetization
diel. polarization

Mori Product

• Mori's scalar product

$$\langle A_\mu | A_\nu \rangle = \int_0^\beta \langle \Delta A_\mu^+(\tau) \Delta A_\nu \rangle d\tau$$

$$\Delta A = A - \langle A \rangle$$

$$A_\mu(\tau) = e^{\tau H} A_\mu e^{-\tau H} \quad \text{imaginary time } \tau \in \mathcal{R}$$

1) bilinear ✓

2) Positive semidefinite

$$\langle A | A \rangle = \int_0^\beta \langle A^+(\tau) A \rangle d\tau = \frac{1}{Z} \sum_{l,m} |\langle l | A | m \rangle|^2 e^{-\beta E_m} \int_0^\beta e^{\tau(E_m - E_l)} d\tau \geq 0 \quad = 0 \Leftrightarrow A=0$$

$$\frac{e^{-\beta E_l} - e^{-\beta E_m}}{E_m - E_l} > 0$$

3) cc-conjugation

$$\langle A_\mu | A_\nu \rangle^* = \int_0^\beta \langle A_\nu^+ A_\mu(-\tau) \rangle d\tau = \langle A_\nu | A_\mu \rangle$$

• isothermal susceptibility

$$\chi_{\mu\nu}^T \equiv \frac{\partial \langle A_\mu^+ \rangle}{\partial f_\nu} = \langle A_\mu | A_\nu \rangle$$

(see tutorial)

↙

Example

(3)

$$b(\tau) = e^{-\omega_0 \tau} b$$

$$b^+(\tau) = e^{\omega_0 \tau} b^+$$

$$\begin{aligned} \Rightarrow \langle + | + \rangle &= \int_0^\beta \langle (e^{-\omega_0 \tau} b + e^{\omega_0 \tau} b^+) (b + b^+) \rangle d\tau \\ &= \int_0^\beta \langle b b^+ \rangle e^{-\omega_0 \tau} d\tau + \int_0^\beta \langle b^+ b \rangle e^{\omega_0 \tau} d\tau \\ &= (1 + n_\beta) \left(-\frac{1}{\omega_0} \right) (e^{-\beta \omega_0} - 1) + n_\beta \left(\frac{1}{\omega_0} \right) (e^{\beta \omega_0} - 1) \\ &= \frac{1}{\omega_0} + \frac{1}{\omega_0} = \frac{2}{\omega_0} \end{aligned}$$

$$\Rightarrow \boxed{X_{T=0} = X^\dagger}$$

Liouville Operator

Linear operator on A_μ

$$L A_\mu(t) = [H, A_\mu(t)]$$

$$\dot{A}_\mu(t) = i L A_\mu(t)$$

$$A_\mu(t) = e^{i L t} A_\mu$$

Liouville is hermitean

$$\langle A | L B \rangle = \langle B | L A \rangle^* = \langle L A | B \rangle$$

$$\begin{aligned} \int_0^\beta d\tau \langle A^+(\tau) L B \rangle = \\ \dots \langle e^{\tau H} A^+ e^{-\tau H} [H, B] \rangle \dots \\ \dots \langle e^{\tau H} [H, A]^+ e^{-\tau H} B \rangle \dots \end{aligned}$$

Kubo's identity

$$\langle A | L B \rangle = \langle [A^+, B] \rangle$$

$$\begin{aligned} \int_0^\beta d\tau \langle A^+(\tau) L B \rangle = \\ \dots \langle e^{\tau L} A^+ L B \rangle = \dots - \langle L e^{\tau L} A^+ B \rangle = \\ \dots - \frac{d}{d\tau} \langle e^{\tau L} A^+ B \rangle = - \langle A^+(\beta) B \rangle + \langle A^+ B \rangle = \langle [A^+, B] \rangle \end{aligned}$$

Laplace trafo of dynamical susceptibility

$$\begin{aligned} \chi_{\mu\nu}(z) &= i \int_0^\infty e^{izt} \langle [A_\mu^+(t), A_\nu] \rangle dt \\ &= i \int_0^\infty \langle [A_\mu^+, e^{i(z-L)t} A_\nu] \rangle dt \\ &= - \langle [A_\mu^+, \frac{1}{z-L} A_\nu] \rangle \end{aligned}$$



Example

$$\langle + | + \rangle = \langle + | b + b^+ \rangle$$

with: $-\frac{1}{\omega_0} L b = b$
 $\frac{1}{\omega_0} L b^+ = b^+$

$$\begin{aligned} \Rightarrow \langle + | + \rangle &= -\frac{1}{\omega_0} \langle + | L b \rangle \\ &\quad + \frac{1}{\omega_0} \langle + | L b^+ \rangle \\ &= -\frac{1}{\omega_0} \langle [b + b^+, b] \rangle \\ &\quad + \frac{1}{\omega_0} \langle [b + b^+, b^+] \rangle \end{aligned}$$

$$= \frac{2}{\omega_0} \quad \approx \quad \boxed{\chi^T = \chi_{iso}}$$

$$\begin{aligned} \boxed{\chi_{++}(z)} &= - \langle [[b + b^+], \frac{1}{z-L} (b + b^+)] \rangle \\ &= - \langle [b, \frac{1}{z-L} b^+] \rangle \\ &\quad - \langle [b^+, \frac{1}{z-L} b] \rangle \\ &= \frac{1}{z - \omega_0} (- \langle [b, b^+] \rangle) \\ &\quad + \frac{1}{z + \omega_0} (- \langle [b^+, b] \rangle) \\ &= \boxed{\frac{1}{\omega_0 - z} - \frac{1}{-\omega_0 - z}} \end{aligned}$$

✓ o.k.
see spectral
rep.

Example $\chi_{IBO} \neq \chi^T$

$$H = \underbrace{BS^2}_H + \underbrace{W(\frac{1}{2})S^2}_{W(\frac{1}{2})}, \quad S = \frac{1}{2}$$

$$L S^2 = 0 \quad \boxed{S^2 \equiv \text{conserved}}$$

$$\begin{aligned} \overline{\langle S^2 | S^2 \rangle} &= \int_0^\beta \langle S^2(\frac{\beta}{2}) S^2 \rangle - \beta \langle S^2 \rangle^2 \\ &= \beta (\langle S^2 \rangle^2 - \langle S^2 \rangle^2) \\ &= \frac{\beta}{4} \frac{1}{\omega^2 (\frac{\beta B}{2})} \end{aligned}$$

$$\begin{aligned} \chi(z) &= \langle [S^2, \frac{1}{z-H} S^2] \rangle \\ &= \frac{1}{z} \langle [S^2, S^2] \rangle \\ &= \boxed{0} \end{aligned}$$

$$\boxed{\chi_{IBO} \neq \chi^T}$$

Relaxation Function

• $t=0$: equilibrium with forces $\neq 0$

$$\rho_D(t=0) = \rho_S(t=0) = \frac{1}{Z} e^{-\beta(H - \sum_{\nu} A_{\nu} f_{\nu})}$$

$t > 0$: switch off forces

$$\frac{d}{dt} \langle A_{\mu}^+(t) \rangle = i \text{Tr} \{ [H, A_{\mu}^+(t)] \rho_D(0) \} =$$

$$i \text{Tr} \{ [\sum_{\nu} A_{\nu} f_{\nu}, A_{\mu}^+(t)] \rho_D(0) \} =$$

$$-i \sum_{\nu} \text{Tr} \{ [A_{\mu}^+(t), A_{\nu}] \rho_D(0) \} f_{\nu}$$

$$\langle A^+(t) \rangle = -i \sum_{\nu} \Phi_{\mu\nu}(t) f_{\nu}$$

$$\Phi_{\mu\nu}(t) = i \Theta(t) \left(\chi_{\mu\nu}^T - \int_0^t \chi_{\mu\nu}(t') dt' \right)$$

• Laplace trafo

$$\int_0^{\infty} \Phi_{\mu\nu}(t) e^{izt} dt =$$

$$\Phi_{\mu\nu}(z) = \frac{1}{z} (\chi_{\mu\nu}(z) - \chi_{\mu\nu}^T)$$

$$\frac{1}{z} \chi_{\mu\nu}(z) = -\frac{1}{z} \langle [A_{\mu}^+, \frac{1}{z-L} A_{\nu}] \rangle$$

$$= \frac{1}{z} \langle A_{\mu} | (-L) \frac{1}{z-L} A_{\nu} \rangle$$

$$= \frac{1}{z} \langle A_{\mu} | (z-L-z) \frac{1}{z-L} A_{\nu} \rangle$$

$$= \frac{1}{z} \langle A_{\mu} | A_{\nu} \rangle - \langle A_{\mu} | \frac{1}{z-L} A_{\nu} \rangle$$

$$\Phi_{\mu\nu}(z) = -\langle A_{\mu} | \frac{1}{z-L} A_{\nu} \rangle$$

...by the way

$$\Phi''_{\mu\nu}(t) = \frac{1}{2} \langle \mathbf{A}_\mu | e^{-i\mathbf{L}t} \mathbf{A}_\nu \rangle$$

spectral function of relaxation function

$$\Phi''_{\mu\nu}(\omega) = \pi \langle \mathbf{A}_\mu | \delta(\omega - \mathbf{L}) \mathbf{A}_\nu \rangle$$

Fouriertrafo

$$\Im \Phi_{\mu\nu}^{\text{R}}(\omega) = \Im \Phi_{\mu\nu}(\omega + i0^+) = -\Im \langle \mathbf{A}_\mu | \frac{1}{\omega + i0^+ - \mathbf{L}} \mathbf{A}_\nu \rangle = \pi \langle \mathbf{A}_\mu | \delta(\omega - \mathbf{L}) \mathbf{A}_\nu \rangle$$

O.K. ✓

$$\chi''_{\mu\nu}(\omega) = \omega \Phi''_{\mu\nu}(\omega)$$

beware if $\mathbf{L} \mathbf{A}_\nu = 0 \Rightarrow$

$$\frac{\chi''_{\mu\nu}(\omega)}{\omega} \neq \Phi''_{\mu\nu}(\omega)$$

Sum Rules and Moments

n-th moment of the spectrum

$$\int \frac{d\omega}{\pi} \omega^n \chi''_{\mu\nu}(\omega) =$$

$$\int \frac{d\omega}{\pi} \omega^{n+1} \Phi''_{\mu\nu}(\omega) =$$

$$\int d\omega \omega^{n+1} \langle A_\mu | \delta(\omega - L) A_\nu \rangle =$$

$$\langle A_\mu | L^{n+1} A_\nu \rangle =$$

$$\langle [A_\mu^+, [H, [H, \dots, A_\nu] \dots]] \rangle$$

n commutators
with H

Typical example: „f sum-rule“

polarization: $d = e x$

$$\int \frac{d\omega}{\pi} \omega \chi''_{xx}(\omega) = \langle [x, [H, x]] \rangle$$

electrons with renorm. mass m^* : $H = \frac{p^2}{2m^*}$

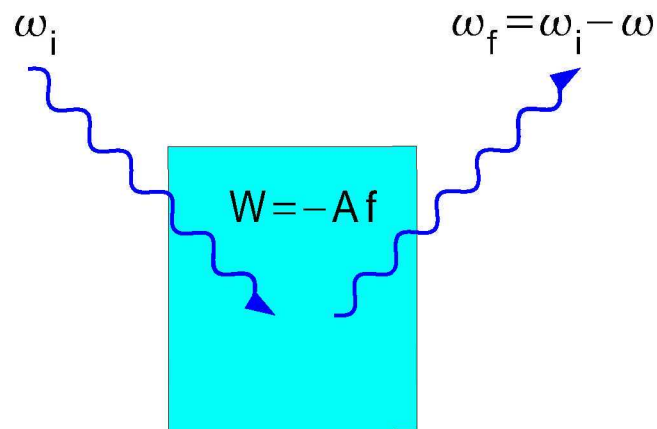
$$\int \frac{d\omega}{\pi} \omega \chi''_{dd}(\omega) = \frac{e^2 \hbar^2}{m^*}$$

spectrum of dielectric susceptibility

similar stuff for optical conductivity

Dynamical Correlation Functions

Scattering: neutrons, light, ...



$|l\rangle \rightarrow |m\rangle$

Intensity from „golden rule“

$$I(\omega) = \frac{2\pi}{Z} \sum_{l,m} e^{-\beta E_l} |\langle m|A|l\rangle|^2 \delta(\omega - E_m + E_l)$$

$$\delta(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} dt$$

$$\dots \frac{1}{Z} \sum_{l,m} \int_{-\infty}^{\infty} e^{i\omega t} e^{-\beta E_l} \langle l|e^{iE_l t} A e^{-iE_m t}|m\rangle \langle m|A|l\rangle dt =$$


$$\dots \frac{1}{Z} \sum_{l,m} \int_{-\infty}^{\infty} e^{i\omega t} e^{-\beta E_l} \langle l|e^{iHt} A e^{-iHt}|m\rangle \langle m|A|l\rangle dt =$$


$$\dots \int_{-\infty}^{\infty} e^{i\omega t} \langle A(t)A \rangle dt$$

$$I(\omega) \propto \int_{-\infty}^{\infty} e^{i\omega t} \langle A(t)A \rangle dt \equiv S_{AA}(\omega) \quad \text{dynamical correlation function}$$

Dissipation and Passivity

$$\tilde{H}_S(t) = H - \sum_{\mu} A_{\mu} f_{\mu}(t)$$


 hermitean


 real

• Rate of energy change

$$\begin{aligned} \frac{dW}{dt} &= \text{Tr}\{\rho_S(t)\dot{\tilde{H}}_S(t)\} + \\ &\quad \text{Tr}\{\dot{\rho}_S(t)\tilde{H}_S(t)\} \\ &= -\sum_{\mu} \langle A_{\mu} \rangle(t) \dot{f}_{\mu}(t) \end{aligned}$$

• Total energy absorbed

$$\begin{aligned} W(\infty) - W(-\infty) &= \\ &\sum_{\mu} \int_{-\infty}^{\infty} f_{\mu}(t) \frac{d\langle A_{\mu} \rangle(t)}{dt} dt = \\ &\sum_{\mu\nu} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f_{\mu}(-\omega) (-i\omega) \chi_{\mu\nu}(\omega) f_{\nu}(\omega) = \end{aligned}$$

$$\sum_{\mu\nu} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f_{\mu}(-\omega) \omega \chi''_{\mu\nu}(\omega) f_{\nu}(\omega)$$

• Dissipative systems

$$\omega \chi''_{\mu\nu}(\omega) = \omega^2 \Phi''_{\mu\nu}(\omega) \geq 0$$

Fluctuation-Dissipation Theorem

• note

$$\begin{aligned} \langle BA \rangle &= \frac{1}{Z} \text{Tr}\{e^{-\beta H} BA\} \\ &= \langle A(\beta)B \rangle = \langle e^{\beta L} AB \rangle \end{aligned}$$

where: $A(x) = e^{xH} A e^{-xH}$

• with 'real' time dependence

$$\begin{aligned} \langle BA(it) \rangle &= \langle e^{(it+\beta)L} AB \rangle \\ \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle BA(it) \rangle dt &= e^{-\beta\omega} \langle \delta(\omega+L) AB \rangle \end{aligned}$$

or

$$\begin{aligned} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle [A(it), B]_{\pm} \rangle dt \\ &= (1 \pm e^{-\beta\omega}) \langle \delta(\omega+L) AB \rangle \\ &= (1 \pm e^{-\beta\omega}) \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{i\omega t} \langle A(it)B \rangle \end{aligned}$$

• Relation between spectrum of dynamical susceptibility and correlation function \equiv relation between dissipation and fluctuation

$$\chi''_{AB}(\omega) = \frac{1}{2} (1 \pm e^{-\beta\omega}) S_{AB}(\omega)$$

• detailed balance

$$\chi''_{AB}(\omega) = -\chi''_{\bar{B}\bar{A}}(-\omega)$$

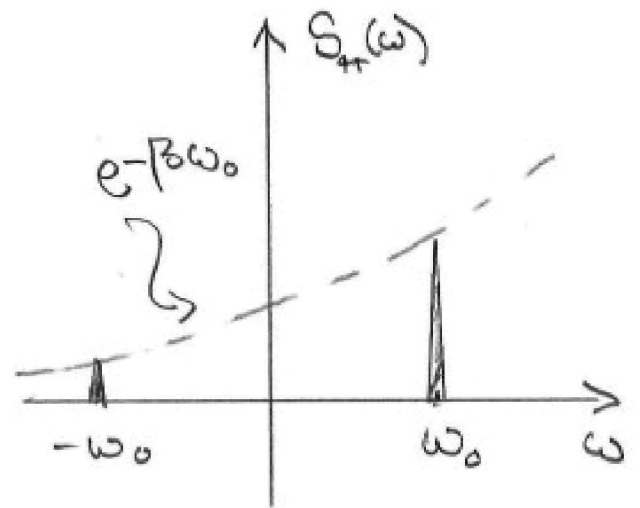
$$e^{-\beta\omega} S_{AB}(\omega) = S_{\bar{B}\bar{A}}(-\omega)$$

Stokes Anti-Stokes



Example

$$\begin{aligned}
S_{rr}(t) &= \langle (e^{-i\omega_0 t} Q + e^{i\omega_0 t} Q^\dagger)(Q + Q^\dagger) \rangle \\
&= e^{-i\omega_0 t} \langle QQ^\dagger \rangle + e^{i\omega_0 t} \langle Q^\dagger Q \rangle \\
&= \underbrace{(1 + n_{\omega_0}) e^{-i\omega_0 t} + n_{\omega_0} e^{i\omega_0 t}}_{\text{is fct. of } T}
\end{aligned}$$



$$\Rightarrow S_{rr}(\omega) = 2\pi [(1+n) \delta(\omega - \omega_0) + n \delta(\omega + \omega_0)]$$

$$\begin{aligned}
\Rightarrow \left(\frac{1}{2} S_{rr}(\omega) \cdot (1 - e^{-\beta\hbar\omega}) \right) &= \pi \left[(1 - e^{-\beta\hbar\omega_0}) \cdot \frac{1}{1 - e^{-\beta\hbar\omega_0}} \delta(\omega - \omega_0) \right. \\
&\quad \left. + (1 - e^{\beta\hbar\omega_0}) \frac{1}{e^{\beta\hbar\omega_0} - 1} \delta(\omega + \omega_0) \right] \\
&= \chi''_{rr}(\omega)
\end{aligned}$$

Projection Technique

• Recursion / 'Dyson' equation

$$\langle A_\mu | \frac{1}{z-L} A_\nu \rangle = [z\mathbf{1} - \mathbf{\Omega} - \mathbf{\Sigma}(z)]^{-1} \chi$$

• Isothermal susceptibility

$$[\chi]_{\mu\nu} = \langle A_\mu | A_\nu \rangle$$

• Frequency term

$$[\mathbf{\Omega} \chi]_{\mu\nu} = \langle A_\mu | \mathbf{L} A_\nu \rangle = \langle [A_\mu^+, A_\nu] \rangle$$

• Memory function

$$[\mathbf{\Sigma}(z) \chi]_{\mu\nu} = \langle \mathbf{L} A_\mu | \mathbf{Q} \frac{1}{z - \mathbf{Q} \mathbf{L} \mathbf{Q}} \mathbf{Q} \mathbf{L} A_\nu \rangle$$

• Projectors

$$\mathbf{P} = \sum_{\mu\nu} |A_\mu\rangle \langle A_\mu | A_\nu \rangle^{-1} \langle A_\nu|; \quad \mathbf{Q} = \mathbf{1} - \mathbf{P}$$

Quicky:

$$1) \frac{1}{z-L} = \frac{1}{z-LQ} (z-L+LP) \frac{1}{z-L} = \frac{1}{z-LQ} + \frac{1}{z-LQ} LP \frac{1}{z-L}$$

$$2) -(1 - \langle A | \frac{1}{z-LQ} \mathbf{L} A \rangle \frac{1}{\langle A | A \rangle}) \phi(z) = \langle A | \frac{1}{z-LQ} A \rangle$$

$$3) -[1 - \frac{1}{z} (\langle A | \mathbf{L} A \rangle + \langle A | \mathbf{L} \mathbf{Q} \frac{1}{z-LQ} \mathbf{L} A \rangle)] \times \frac{1}{\langle A | A \rangle} \phi(z) = \frac{1}{z} \langle A | A \rangle$$

Applications of the Projection Technique ...

... another lecture ...

... and one of the tutorials ...

Finito !