$$
\begin{tikzcd}
\dfrac{d^4\sigma}{d^3\varkappa\, d\omega} \arrow[r, "\text{EXPERIMENT}"'] & \boxed{S(\vec{\varkappa},\omega)} \arrow[r, "\text{THEORY}"'] \arrow[d, "F_\omega"'] & (1+n(\omega))\,\chi''(\vec{\varkappa},\omega) \\
& \langle B^+_{\vec{\varkappa}}(0)\, B_{\vec{\varkappa}}(t)\rangle_T \arrow[d, "F_{\varkappa}"'] & \\
& \int d^3x' \,\langle \tilde{B}(\vec{x}-\vec{x}',0)\,\tilde{B}(\vec{x}',t)\rangle_T = G(\vec{x},t) &
\end{tikzcd}
$$

"SUSCEPTIBILITY"

(Im-PART)

$$B_{\varkappa}(t) = \sum_j e^{-i\varkappa \vec{X}_j(t)}\, b_j$$

$$B^+_{\vec{\varkappa}} = B_{-\vec{\varkappa}}$$

CORRELATION-FCT. (van Hove)

$$G(\vec{x},t) = G^*(-\vec{x},-t)$$

THERMAL AVERAGE $\langle \quad \rangle_T$

– CANONICAL ENSEMBLE

SAMPLE: THERMODYN. EQUILIBRIUM

TEMPERATURE T, $\beta = 1/kT$

PARTITION FCT.: $e^{-\beta F} = \mathrm{Sp}\, e^{-\beta H} = Q$

EXPECTATION VALUE OF AN OBSERVABLE $\hat{O}$ $\quad \langle \hat{O}\rangle_T = \frac{1}{Q}\,\mathrm{Sp}(e^{-\beta H}\hat{O})$

$$\langle \hat{O}\rangle_T = e^{\beta F}\,\mathrm{Sp}(e^{-\beta H}\hat{O}) = \sum_n p_n \langle n|\hat{O}|n\rangle$$

WITH $p_n = e^{-\beta(\hbar\omega_n - F)}$; $\sum_n p_n = 1$

SCATT. PROCESS $\longrightarrow$ ISENTROPIC

INTERACTION HAMILTONIAN

GENERAL FORM

$$H = H_0 + H_1(t)$$

H_0 : INCIDENT FIELD
FREE SAMPLE

H_1 : INTERACTION WITH SAMPLE

$$\boxed{H_1 = \int d^3x \, a(\vec{x},t) \, J(\vec{x})}$$

a : EXT. "POTENTIAL" – SCALAR, SPINOR
VECTOR –
DEPEND. ON PROBE

J : COUPLING BETWEEN PROBE - SAMPLE
– DENSITY, CHARGE-DENS., MAGN.-DENS.
CURRENT - DENS.

ELECTRO-MAGNETIC

$$H_1 = \frac{e}{c} \int d^3x \, \vec{A}(\vec{x},t) \, \vec{j}(\vec{x})$$

$$\vec{j}(\vec{x}) = \sum_i \frac{1}{2m} \left(\vec{p}_i \, \delta(\vec{x}-\vec{X}_i) + \delta(\vec{x}-\vec{X}_i) \, \vec{p}_i \right)$$

IN PRESENCE OF $\vec{A}$: $\vec{p}_i \longrightarrow \vec{p}_i - \frac{e}{m} \vec{A}(\vec{X}_i)$

NEUTRON - MAGNETIC

$$H_1 = \mu_B \int d^3x \, \vec{B}(\vec{x},t) \, \vec{m}(\vec{x}) \qquad \vec{B} = -\gamma \frac{\mu_N}{c} \vec{\nabla} \wedge \left(\vec{\sigma}_N \wedge \vec{\nabla} \frac{1}{|\vec{x}|} \right)$$

i) SPIN $\qquad \vec{m}(\vec{x}) = 2 \sum_i \vec{S}_i^{(e)} \, \delta(\vec{x} - \vec{X}_i)$

ii) ORBITAL CURRENT $\qquad \vec{m}(\vec{x}) = \sum_i (\vec{x} \wedge \vec{p}_i) \, \delta(\vec{x} - \vec{X}_i)$

NEUTRON - NUCLEAR (NOT NUCL. MAGNETISM)

$$H_1 = \sum_i \left[A + B \left(\vec{\sigma}_N \cdot \vec{I}_i \right) \right] \int d^3x \, \psi_\sigma(\vec{x},t) \, \rho(\vec{x})$$

NO UNIVERSAL COUPLING $\qquad \rho(\vec{x}) = \delta(\vec{x} - \vec{X}_i)$

LINEAR RESPONSE

HAMILTONIAN : $H = H_0 + H_1(t)$. H_0 : SAMPLE ! (UNPERTURBED)

$$i\hbar \partial_t \rho = [H, \rho]$$

DYNAMICS IN DIRAC - (INTERACTION) REPRESENTATION

i) OPERATORS DETERM. BY H_0 : $\hat{O}(t) = e^{i/\hbar H_0 t} \hat{O} e^{-i/\hbar H_0 t}$

ii) STATES DETERMINED BY H_1 : $i\hbar \partial_t \rho_I = [H_1^{(I)}(t)\, \rho_I]$

$$\rho = \sum_m p_m |m\rangle\langle m|$$

$$\rho^{(I)}(t) = \rho(0) - \frac{i}{\hbar}\int_{-\infty}^{t} d\tau [H_1^{(I)}(\tau), \rho_0] - \frac{1}{\hbar^2}\int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' [H_1^{(I)}(\tau')[H_1^{(I)}(\tau)\rho_0]] + \dots + O(H_1^3)$$

$\downarrow O(H_1)$

LINEAR RESPONSE

FOR ANY OBSERVABLE $\hat{O}$

$$\langle \hat{O} \rangle_T = Sp(\hat{O}^{(I)}(t)\rho_0) - \frac{i}{\hbar}\int_{-\infty}^{t} d\tau\, Sp(\hat{O}^{I}(\tau)[H_1^{(I)}(\tau), \rho_0])$$

OR

$$\boxed{\langle \delta\hat{O} \rangle_T = -\frac{i}{\hbar}\int_{-\infty}^{t} d\tau \langle [\hat{O}^{(I)}(t)\, H_1^{(I)}(\tau)] \rangle_T \quad \text{WITH } \rho_0 \sim e^{-\beta H_0}}$$

e.g. ELECTRO - MAGNET. PERTURBATION

$$H_1^{(I)}(\tau) = \int d^3x\, J_\mu(x)\, a^\mu(x)$$

$$\boxed{\langle \delta J_\rho \rangle_T = \int d^4x'\, K_{\rho\mu}(x-x')\, a^\mu(x')}$$

RETARDED RESPONSE KERNEL $\longrightarrow -\frac{i}{\hbar}\Theta(x_0 - x_0')\langle [J_\rho^+(x) J_\mu(x')] \rangle_T$

EXTERN. FIELD OF PROBE : $a^\mu(x)$

a : i) POTENTIAL OF ELECTR. MAGN. FIELD
(SYNCHR. RADIATION , X-RAYS)

ii) POTENTIAL OF MAGN. DIPOL
(NEUTRONS)

iii) SPINOR OR SCALAR - WAVE FCT.
(NEUTRONS)

$\theta(x_0 - x_0')$ TAKES CARE OF CAUSALITY
RETARDATION : $\boxed{\text{OUTPUT LATER THEN INPUT}}$

$$\langle [J_\beta^+(x) J_\mu(x')] \rangle_T = \frac{1}{2i} \, \mathrm{Im} \, \langle J_\beta^+(x) J_\mu(x') \rangle_T$$

Im - PART OF CORREL.-
FUNCTION OF " CURRENT " -
FLUCTUATIONS

e.g. FOR NUCLEAR NEUTRON SCATTERING

$$\langle \tilde{\rho}_{\vec{x}}(0) \, \tilde{\rho}^+_{\vec{x}}(\tau) \rangle_T \xrightarrow[\mathrm{Im-PART}]{} \langle [\tilde{\rho}_{\vec{x}}(0) \tilde{\rho}^+_{\vec{x}}(\tau)] \rangle_T$$

$$\Big\downarrow \text{RETARDATION}$$

$$\theta(\tau) \langle [\tilde{\rho}_{\vec{x}}(0) \tilde{\rho}^+_{\vec{x}}(\tau)] \rangle_T$$

$$\langle [\rho_{\vec{x}}(0) \rho^+_{\vec{x}}(\tau)] \rangle_T \xrightarrow[\mathcal{F}_T^{-1}]{} (1 - e^{-\hbar\omega \cdot \beta}) \, S(\vec{x}, \omega)$$

$$\theta(\tau) \langle [\rho_{\vec{x}}(0) \rho^+_{\vec{x}}(\tau)] \rangle_T \xrightarrow[\mathcal{F}_T^{-1}]{} \, ?$$

GENERALIZED
SUSCEPTIBILITY

Re - PART $\longleftrightarrow$ Im - PART

$$\boxed{[1+n(\omega)]\,\mathrm{Im}\,\tilde{K}(\omega,\vec{x}) = \pi S(\omega,\vec{x})}$$

$$1+n(\omega) = (1-e^{-\beta\hbar\omega})^{-1}$$

$$n(\omega) = \frac{1}{e^{\beta\hbar\omega}-1}$$

REMINDER :

$\mathrm{Im}\,Y$: $\langle[\tilde{\rho}_x(0)\rho_x^+(\tau)]\rangle_T$

$$= \langle \tilde{\rho}_x(0)\rho_x^+(\tau) - \rho_x^+(\tau)\rho_x(0)\rangle_T$$

$$\tilde{\rho}_x(0)\rho_x^+(\tau) \xrightarrow{\mathcal{F}^{-1}} S(\omega,\vec{x}) \qquad \rho_x^+(\tau)\rho_x(0) \xrightarrow{\mathcal{F}^{-1}} S(\omega,\vec{x})\,e^{-\beta\hbar\omega} = S(-\omega,\vec{x})$$

$$\mathrm{Im}\,\tilde{K}(\omega,\vec{x}) \sim (S(\omega,\vec{x}) - S(-\omega,\vec{x}))$$

ENERGY : IN OUT

$\mathrm{Im}\,\tilde{K}$: ABSORPTIVE PART OF GENERALIZED SUSCEPTIBILITY

$S(-\omega,\vec{x})$ ONLY RELEVANT FOR THERMALLY EXCITED SAMPLES ($T \neq 0$) ("ANTI-STOKES")

ω-INTERVAL ($\lesseqgtr 0$) WITH $\mathrm{Im}\,\tilde{K} \neq 0$ DEPENDS ON $\vec{x}$ (SEE PLOT FOR KINEMAT. ACCSESS).

S (DIFF. CROSS-SECTION) $\longrightarrow$ DETERMINES $\mathrm{Im}\,\tilde{K}^R$

? WHAT ABOUT $\mathrm{Re}\,\tilde{K}^R$?

CAUSALITY COND. OF LINEAR RESPONSE $\longleftarrow$

DISPERSION RELATIONS $\longrightarrow$ KRAMERS KRONIG

WRITE

$$\phi(\tau) = \langle [\tilde{\rho}_x(0)\, \tilde{\rho}_x^+(\tau)] \rangle_T = \mathrm{Im} \langle \rho_x(0)\, \rho_x^+(\tau) \rangle_T$$

$$\boxed{\begin{array}{c}\text{ANTISYM. IN } \tau \\ -\phi(\tau) = \phi(-\tau)\end{array}}$$

$$\tilde{K}^R(\omega) = \int_{-\infty}^{+\infty} d\tau\, e^{-i\omega\tau}\, \Theta(\tau)\, \phi(\tau)$$

USE

$$\frac{1}{2\pi i} \lim_{\varepsilon \to 0} \int_{-\infty}^{+\infty} d\xi\, e^{i\xi\tau} \frac{1}{\xi - i\varepsilon}$$

$$\frac{1}{2\pi i} \int_{-\infty}^{+\infty} d\tau \int_{-\infty}^{+\infty} d\xi\, \frac{e^{i\tau(\xi-\omega)}}{\xi - i\varepsilon}\, \phi(\tau)$$

SUBSTITUTE

$$\xi \longrightarrow \omega - \xi \qquad \frac{e^{-i\xi\tau}}{\omega - \xi - i\varepsilon}$$

FROM ANTISYM. OF $\phi(\tau)$

$$\int_{-\infty}^{+\infty} e^{-i\xi\tau} \phi(\tau)\, d\tau = -2i \int_0^{\infty} d\tau\, \sin(\xi\tau)\, \phi(\tau) = -2i\, \chi''(\omega) \sim S(\omega, \vec{x})$$

AND

$$\lim_{\varepsilon \to 0} \frac{1}{\eta - i\varepsilon} = P\left(\frac{1}{\eta}\right) + i\pi\, \delta(\eta)$$

$$\chi(\omega) = \int_{-\infty}^{+\infty} \frac{d\xi\, \chi''}{\omega - \xi - i\varepsilon} = i \int_{-\infty}^{+\infty} d\xi\, \delta(\omega - \xi)\, \chi''(\xi) + \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\chi''(\xi)}{\omega - \xi}\, d\xi$$

KRAMERS - KRONIG (DISPERSION) - RELATIONS FOLLOW :

$$\boxed{\begin{aligned} \chi'(\omega) &= \frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\chi''(\omega)}{\omega - \xi}\, d\xi \\ \chi''(\omega) &= -\frac{P}{\pi} \int_{-\infty}^{+\infty} \frac{\chi'(\omega)}{\omega - \xi}\, d\xi \end{aligned}} \qquad \tilde{K}^{(R)}(\omega) = \chi'(\omega) + i\chi''(\omega)$$

THIS IS A CONSEQUENCE OF CAUSALITY (RETARDATION)

HENCE :

Im PART KNOWN (MEASURED) $\longrightarrow$ Re - PART

THE RETARDED KERNEL (RESPONSE) IN THE LEHMANN REPRESENTATION

$$K^{(R)}_{\alpha\beta}(x) = -\frac{i}{\hbar}\,\theta(x_0)\,\langle [J^{+}_{\alpha}(x) J_{\beta}(0)] \rangle_T$$

$\downarrow$ $\mathcal{F}$ - TRANSFORM

$$\tilde{K}^{(R)}_{\alpha\beta}(k) = \left(\frac{1}{2\pi}\right)^2 \int d^4x\, K^{(R)}_{\alpha\beta}(x)\, e^{ikx}$$

USE
i.) INTEGR. REPRESENT. OF $\theta(x_0)$
ii) EXTENSION (TRANSL. INV.)
$\tau \longrightarrow \tau + i\beta\hbar$

THEN

$$\mathrm{Im}\,\tilde{K}_{\alpha\beta}(\omega, \vec{\kappa}) \sim \sum_{m,n} \delta^{(3)}(\vec{\kappa} - \vec{k}_m - \vec{k}_n)\, e^{-\beta(\hbar\omega_{mn} - F)} (1 - e^{-\beta\hbar\omega_{mn}})$$

$$\times \langle m | J^{+}_{\alpha} | n \rangle \langle n | J_{\beta} | m \rangle\, \delta(\omega - \omega_{mn})$$

$\sum_{m,n} e^{\beta F}$ — $\frac{1}{Q}\,\mathrm{Sp}(\quad)$

$J^{+}_{\alpha} J_{\beta}$ $\longrightarrow$ $A^{mn}_{\alpha\beta}$: TRANSITION PROBAB. $W_{m \to n}$

$$\mathrm{Im}\,\tilde{K}_{\alpha\beta}(\omega) \sim \sum_{m,n} (p_m - p_n)\, w_{m \to n} \sim (S(\omega) - S(-\omega))$$

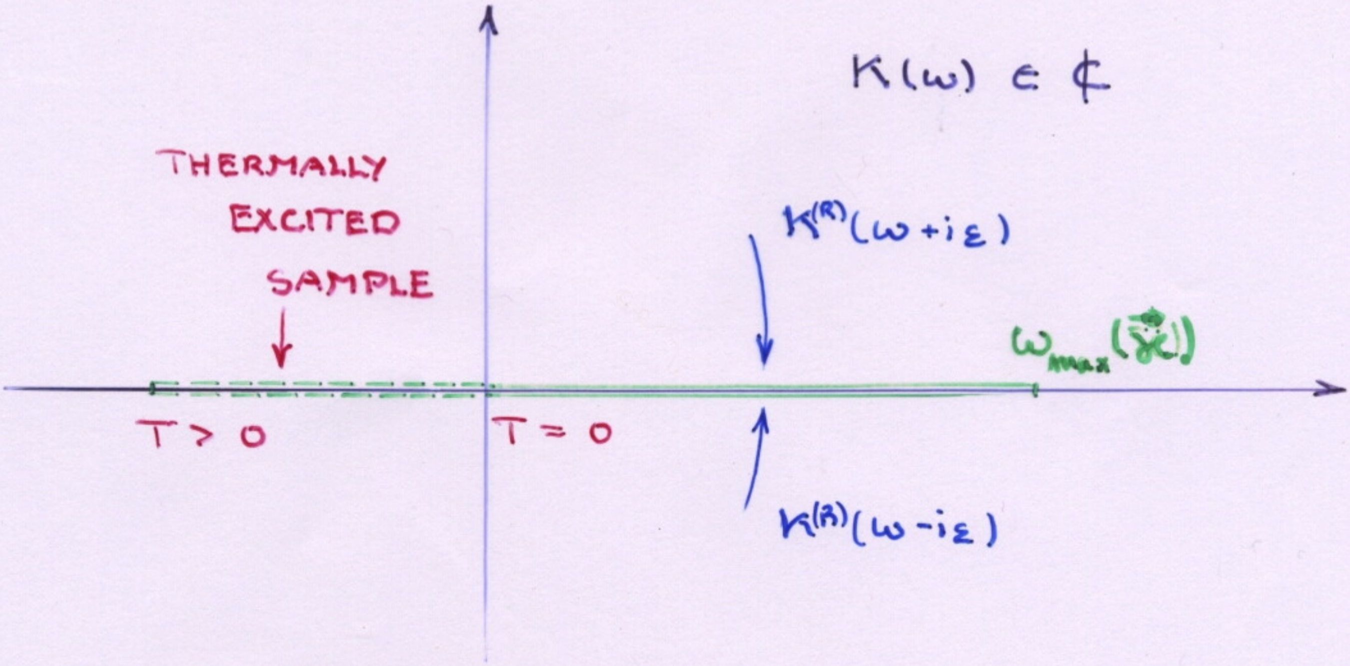
ENERGY: IN OUT

$\downarrow$ WRITE

$\rho(\omega)$; AND USE KRAMERS - KRONIG

$$\boxed{K^{R}(\omega) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{d\omega'\, \rho(\omega')}{(\omega' - \omega) - i\varepsilon}}$$

LEHMANN SPECTRAL REPRESENTATION

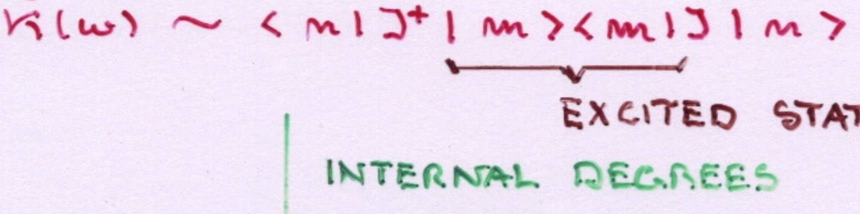


$$K^R(\omega+i\varepsilon) - K^R(\omega-i\varepsilon) = \mathrm{Im}\,K^R(\omega) \sim \delta(\omega-\omega')$$

DISC. $\rho(\omega)$ ON Re-AXIS $\sim S(\omega,\vec{\kappa})$

PHYS. CROSS-SECTION

INTERNAL DEGREES OF FREEDOM OF THE SAMPLE CONTRIBUTE TO THE SPECTRAL FUNCTION $\rho(\omega)$



$$\mathrm{Im}\,\tilde{K}(\omega) \sim \langle n|J^+\underbrace{|m\rangle\langle m|}_{\text{EXCITED STATES OF SPECIMEN}}J|n\rangle$$

INTERNAL DEGREES OF FREEDOM

FLUCTUATIONS OF UNPERTURBED SAMPLE $\longleftrightarrow$ RESPONSIBLE FOR ENERGY TRANSFER TO PERTURBED SAMPLE (DISSIPATION)

FLUCTUATION

TIME CORRELATION :

$$\varphi(t'-t) = \langle J(t')\, J^{+}(t) \rangle$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \int_{-\infty}^{+\infty} d\omega' \,\langle \tilde{J}(\omega')\, \tilde{J}^{+}(\omega)\rangle\, e^{i(\omega t + \omega' t')}$$

Q.M. (NOT - C - NB.)

$$\boxed{\langle \{ \tilde{J}(\omega)\, J^{+}(\omega') \} \rangle_T}$$

POWER - SPECTR. OF FLUCTUATION

FROM INVARIANCE UNDER t - TRANSL.

$$\langle \{ \tilde{J}(\omega)\, \tilde{J}^{+}(\omega') \} \rangle_T \sim \delta(\omega + \omega')$$

DEFINITION : $\langle J^2 \rangle_\omega$

$$\frac{1}{2} \langle \tilde{J}(\omega)\tilde{J}^{+}(\omega') + \tilde{J}^{+}(\omega')\tilde{J}(\omega) \rangle_T = 2\pi \langle J^2 \rangle_{\omega,T}\, \delta(\omega + \omega')$$

SAME PROCEDURE AS FOR COMMUTATOR LEADS TO :

$$\boxed{\langle J^2 \rangle_{\omega,T} = \hbar \,\mathrm{Cth}\left(\frac{\hbar\omega}{2kT}\right) \mathrm{Im}\, \tilde{K}(\omega)}$$

SQUARED FLUCTUATION OF UNPERTURBED SYSTEM IN THERMAL EQUILIBRIUM

LINEAR DISSIPATIVE RESPONSE TO AN EXTERNAL PERTURB.

$$\mathrm{Cth}\left(\frac{\hbar\omega}{2kT}\right) \begin{cases} \to 1 & kT \ll \hbar\omega \\ \to \infty & kT \gg \hbar\omega \end{cases}$$

$$\frac{1}{2}\,\frac{1 + e^{-\hbar\omega/kT}}{1 - e^{-\hbar\omega/kT}} = \left\{ \frac{1}{2} + \frac{1}{e^{\hbar\omega/kT} - 1} \right\}$$

ZERO POINT ENERGY

ENERGY CONTENT OF SAMPLE