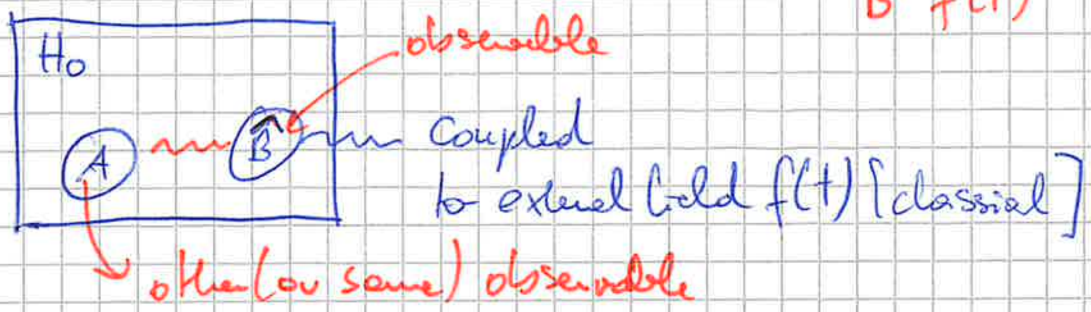
1.3 linear response theory

physical situation: $$H(t) = \overset{\text{unperturbed time-independent}}{H_0} + B(t) \leftarrow \text{perturbation}$$

$$B(t) = \hat{B}\, f(t)$$



in the experiment we measure

$$\delta\langle A(t)\rangle = \langle A\rangle_{H(t)} - \langle A\rangle_{\substack{H_0 \\ (B(t)=0)}} = \text{response of system to external perturbation}$$

How can we calculate this response?

Kubo(*)-Nakano formula

(*) R. Kubo (1920-1995)

linear response: $$\delta\langle A(t)\rangle \propto f(t) = \int_{-\infty}^{\infty} dt'\, \underset{\displaystyle \| \atop \displaystyle C_{AB}(t,t')}{\chi_{AB}(t,t')}\, f(t')$$

χ_{AB}/C_{AB} ... susceptibility / correlation function

$$\langle A\rangle_{H_0} = \frac{1}{Z_0}\mathrm{Tr}[\rho_0 A] = \frac{1}{Z_0}\sum_n \langle \overset{\text{eigenstates}}{n}|A|n\rangle\, e^{-\beta \overset{\text{EVs}}{E_n}}$$

$$Z_0 = \mathrm{Tr}[\rho_0],\quad \rho_0 = e^{-\beta H_0} = \sum_n |n\rangle\langle n|\, e^{-\beta E_n} \text{ ... density operator}$$

at $t = t_0$ we switch on the perturbation:

$$H(t) = H_0 + B(t)\,\Theta(t-t_0)$$

$$\langle A(t)\rangle = \frac{1}{Z_0}\sum_n \langle n(t)|A|n(t)\rangle\, e^{-\beta E_n} = \frac{1}{Z_0}\mathrm{Tr}[\rho(t) A]$$

$$\rho(t) = \sum_n |n(t)\rangle\langle n(t)|\, e^{-\beta E_n}$$

philosophy: initial states are distributed according to usual Boltzmann $e^{-\beta E_{0n}}/Z_0$

later: same distribution, but states evolved according to $H(t)$

$$i\partial_t |n(t)\rangle = H(t)|n(t)\rangle$$

interaction picture: $|n(t)\rangle = e^{-iH_0 t}|\hat{n}(t)\rangle = e^{-iH_0 t}\hat{U}(t,t_0)|\hat{n}(t_0)\rangle$

linear order in $B(t)$: $\hat{U}(t,t_0) = 1 - i\int_{t_0}^{t} dt'\, \hat{B}(t')$

$$\Rightarrow \langle A(t)\rangle_{H(t)} = \frac{1}{Z_0}\sum_n \langle n(t)|A|n(t)\rangle e^{-\beta E_n} =$$

$$= \frac{1}{Z_0}\sum_n e^{-\beta E_n}\langle n(t_0)|\underbrace{\hat{U}(t,t_0)}_{1+i\int_{t_0}^{t} dt'\hat{B}(t')} e^{iH_0 t} A e^{-iH_0 t}\underbrace{\hat{U}(t,t_0)}_{1-i\int_{t_0}^{t} dt'\hat{B}(t')}|n(t_0)\rangle =$$

$$= \left|\begin{matrix}\text{keep only linear}\\ \text{terms in } B\end{matrix}\right| = \langle A\rangle_{H_0} +$$

$$- i\int_{t_0}^{t} dt'\, Z_0 \sum_n \underset{\infty}{e^{-\beta E_n}}\langle n(t_0)|\hat{A}(t)\hat{B}(t') - \hat{B}(t')\hat{A}(t)|n(t_0)\rangle$$

"retarded"

$$\Rightarrow \boxed{\delta\langle A(t)\rangle = \int_{t_0} dt'\, C^R_{AB}(t,t') \quad \text{with } C^R_{AB}(t,t') = -i\Theta(t-t')\langle[\hat{A}(t),\hat{B}(t')]\rangle_{\textcircled{H_0}}\ !!!}$$

Kubo-Nakano formula

$$\text{if } \hat{B}(t) = B f(t) \qquad \Rightarrow C_{AB}(t,t') = C_{AB}(t-t')f(t')$$

not time-dependent

no operator

general properties of C^R_{AB}:

·) causality: $C^R_{AB}(t-t') = \Theta(t-t')\, C^R_{AB}(t-t')$

·) finiteness in time: $|C^R_{AB}(t-t')| <$ const. $\forall t, t'$

·) Fourier transform

$$C^R_{AB}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, C^R_{AB}(t)$$

integrand must decay for $t-t' \to \infty$ (no correlations)

However: relaxation mechanisms that destroy correlations not necessarily given (e.g. non-interacting case)

way out: perform F.T. with complex frequency $\omega + i\eta$ $(\eta \to 0^+)$

$$C^R_{AB}(\omega) = C^R_{AB}(z = \omega + i0^+) = \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} dt\, C_{AB}(t)\, e^{i(\omega + i\eta)t}$$

$$\Rightarrow \delta\langle A(\omega)\rangle = C^R_{AB}(\omega)\, f(\omega)$$

·) Kramers - Kronig relations

$$\mathrm{Re}\, C_{AB}(\omega) = \frac{1}{\pi} P \int d\tilde{\omega}\, \frac{\mathrm{Im}\, C_{AB}(\tilde{\omega})}{\tilde{\omega} - \omega}$$

$$\mathrm{Im}\, C_{AB}(\omega) = -\frac{1}{\pi} P \int d\tilde{\omega}\, \frac{\mathrm{Re}\, C_{AB}(\tilde{\omega})}{\tilde{\omega} - \omega}$$

examples: see slides