Fluktuations-Dissipations-Theorem

Kubo Formel $V = -\int d^3r\, F(\vec r, t)\, \hat A(\vec r)$ $\quad \langle \delta B(\vec r, t)\rangle = \int dt'\, d^3r'\, \chi_{BA}(\vec r - \vec r', t - t')\, F(\vec r, t)$

Response-Fkt $\chi_{BA}(\vec r - \vec r', t - t') = \frac{i}{\hbar} Tr(\rho_0 [B_I(\vec r, t), A_I(\vec r', t')])\, \Theta(t - t')$

$$= \frac{i}{\hbar} \langle [B(r,t), A(r',t')] \rangle_0\, \Theta(t-t')$$

Gleichgewichts-Dichte-Matrix $\rho_0 = \frac{1}{Z_0} \exp[-\frac{H_0}{k_B T}]$ $\quad \uparrow$ im Gleichgewicht

$B = B_I = B_H$ wenn $H = H_0$

$\boxed{H_0 |n\rangle = E_n |n\rangle \quad \text{Vollst. Satz}}$ $\quad \sum_{n'} |n'\rangle\langle n'| = \mathbb{1}$

B=A $\chi_{AA} = \frac{i}{\hbar} \frac{\Theta(t-t')}{Z_0} \sum \langle n| e^{-\beta H_0} [A(t), A(t')] |n\rangle$

$$= \frac{i}{\hbar} \frac{\Theta(t-t')}{Z_0} \sum_n \left(\langle n| e^{-\beta H_0} e^{\frac{i}{\hbar} H_0 t} A_s(r) e^{-\frac{i}{\hbar} H_0 t} e^{\frac{i}{\hbar} H_0 t'} A_s(r') e^{-\frac{i}{\hbar} H_0 t'} |n\rangle - \begin{matrix} r \leftrightarrow r' \\ t \leftrightarrow t' \end{matrix} \right)$$

$\boxed{A(t) = e^{\frac{i}{\hbar} H_0 t} A_s e^{-\frac{i}{\hbar} H_0 t}}$

$$= \frac{i}{\hbar} \frac{\Theta(t-t')}{Z_0} \sum_{nn'} \left(\langle n| A_s(r) |n'\rangle \langle n'| A_s(r') |n'\rangle e^{-\beta E_n} e^{\frac{i}{\hbar} E_n (t-t')} e^{-\frac{i}{\hbar} E_{n'}(t-t')} - \begin{matrix} r \leftrightarrow r' \\ t \leftrightarrow t' \end{matrix} \right)$$

Fouriertrafo $(t \to \omega)$ $\quad \int_0^\infty dt\, e^{i\omega t} e^{-\delta t} = \frac{1}{-i\omega + \delta} = i \frac{1}{\omega - i\delta} = i\left(PV\frac{1}{\omega} - i\pi\delta(\omega)\right)$

Hauptwert $\hat=$ PV (prinzipal Value)

$\chi(r, r', \omega) = \int_{-\infty}^{\infty} d\tau\, \chi(r, r', \tau) e^{i\omega\tau}$ $\quad$ mit $\tau = t - t'$ $\quad \left(\text{mit } \Theta\text{-Fkt } \int_{-\infty} \to \int_0\right)$

$$= \frac{i}{\hbar} \frac{1}{Z_0} \sum_{nn'} \left(\langle n| A_s(r) |n'\rangle \langle n'| A_s(r') |n\rangle \frac{i\, e^{-\beta E_n}}{\omega + \frac{E_n - E_{n'}}{\hbar} + i\delta} - \langle n| A_s(r') |n'\rangle \langle n'| A_s(r) |n\rangle \frac{i\, e^{-\beta E_n}}{\omega + \frac{E_{n'} - E_n}{\hbar} + i\delta} \right)$$

$\chi(k, \omega) = \int d^3(r - r')\, \chi(r - r', \omega)\, e^{-ik(r - r')}$ $\quad$ | $\quad A(r), A(r') \longrightarrow A$

$$\chi(\omega) = -\frac{1}{\hbar Z_0} \sum_{nn'} |\langle n|A|n'\rangle|^2 e^{-\beta E_n} \left(\frac{1}{\omega + \frac{E_n - E_{n'}}{\hbar} + i\delta} - \frac{1}{\omega + \frac{E_{n'} - E_n}{\hbar} + i\delta} \right)$$

$Re(\chi) = \chi'$, $\; Im(\chi) = \chi''$, $\; \chi = \chi' + i\chi''$

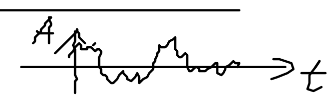
$$\chi'' = \frac{\pi}{\hbar Z_0} \sum_{nn'} |\langle n|A|n'\rangle|^2 e^{-\beta E_n} \left(\delta(\omega + \frac{E_n - E_{n'}}{\hbar}) - \delta(\omega - \frac{E_n - E_{n'}}{\hbar}) \right)$$

$$= \frac{\pi}{\hbar Z_0} \sum_{nn'} |\langle n|A|n'\rangle|^2 \delta(\omega + \frac{E_n - E_{n'}}{\hbar}) \left(e^{-\beta E_n} - e^{-\beta E_{n'}} \right)$$

$\boxed{\frac{E_n - E_{n'}}{\hbar} = -\omega \quad E_{n'} = E_n + \hbar\omega}$

$$\boxed{\chi'' = \frac{\pi}{\hbar Z_0} e^{-\beta E_n} (1 - e^{-\beta\hbar\omega}) \sum_{nn'} |\langle n|A|n'\rangle|^2 \delta(\omega + \frac{E_n - E_{n'}}{\hbar})}$$

Korrelations-Fkt $\langle A(t) A(t') \rangle = Tr(\rho_0 A(t) A(t'))$ $\quad \langle A \rangle = 0$



Rauschen $S(t - t') = \langle A(t) A(t') + A(t') A(t) \rangle$ symmetrisierte Korrelations-Fkt weißes Rauschen (Frequenzunabhängig) $\langle A(t)A(t')\rangle \sim \delta(t-t')$

$$S(t-t') = \frac{1}{2}\sum_n \left(\langle n|\frac{1}{Z_0}e^{-\beta H_0} e^{\frac{i}{\hbar}H_0 t} A e^{-\frac{i}{\hbar}H_0 t} e^{\frac{i}{\hbar}H_0 t'} A e^{-\frac{i}{\hbar}H_0 t'}|n\rangle + t \leftrightarrow t'\right)$$

$$= \frac{1}{2Z_0}\sum_{nn'}\left(|\langle n|A|n'\rangle|^2 e^{-\beta E_n} e^{\frac{i}{\hbar}(E_n-E_{n'})(t-t')} + t\leftrightarrow t'\right)$$

$$S(\omega) = \frac{1}{Z_0}\sum_{nn'}|\langle n|A|n'\rangle|^2 e^{-\beta E_n}\left(2\pi\delta\left(\omega+\frac{E_n-E_{n'}}{\hbar}\right)+2\pi\delta\left(\omega-\frac{E_n-E_{n'}}{\hbar}\right)\right) \qquad \boxed{\int_{-\infty}^{\infty} dt\, e^{i\omega t} = 2\pi\delta(\omega)}$$

$$= \frac{\pi}{Z_0}\left(1+e^{-\beta\hbar\omega}\right)e^{-\beta E_n}\sum_{nn'}|\langle n|A|n'\rangle|^2\delta\left(\omega+\frac{E_n-E_{n'}}{\hbar}\right)$$

$$\boxed{S(\omega) = \hbar\coth\left(\frac{\beta\hbar\omega}{2}\right)\chi''(\omega)}$$ **Fluktuations-Dissipations-Theorem**

- ist das Rauschen messbar, kann man die Response Fkt bestimmen
- Dissipation $\hat{=}$ Im(Response-Fkt)

$\coth x \approx \frac{1}{x} \quad x \ll 1$ $\qquad$ $\hbar\omega \ll k_B T$ (klassisch) $\Rightarrow S(\omega) \approx \frac{2}{\omega\beta}\chi''(\omega) = \frac{2k_BT}{\omega}\chi''(\omega)$

$\chi(t-t') \sim \Theta(t-t') \Rightarrow \chi(\omega)$ Analytisch für $\mathrm{Im}(\omega) > 0$

$\chi(\tau) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{-i\omega\tau}\chi(\omega) \qquad \chi(\tau<0) = 0 \Rightarrow \omega = i\alpha,\ \alpha>0 \Rightarrow e^{\alpha\tau}$

$$\left.\begin{aligned} \chi'(\omega) &= \frac{PV}{\pi}\int d\omega'\,\frac{\chi''(\omega')}{\omega'-\omega} \\ \chi''(\omega) &= -\frac{PV}{\pi}\int d\omega'\,\frac{\chi'(\omega')}{\omega'-\omega} \end{aligned}\right\} \text{Kramers-Kronig-Relation}$$