

Fluktuation - Dissipationstheorem

Kubo-Formel $V = - \int d\vec{r} F(\vec{r}, t) \hat{A}(\vec{r})$

$$\langle \delta B(\vec{r}, t) \rangle = \int dt' d\vec{r}' \chi(\vec{r} - \vec{r}', t - t') F(\vec{r}', t')$$

$$\begin{aligned} \chi_{BA}(\vec{r} - \vec{r}', t - t') &= \frac{i}{\hbar} \text{Tr} \left\{ \rho_0 [B_I(\vec{r}, t), A_I(\vec{r}', t')] \right\} \Theta(t - t') \\ &= \frac{i}{\hbar} \langle [B(\vec{r}, t), A(\vec{r}', t')] \rangle_0 \Theta(t - t') \end{aligned}$$

Hessenberg $\rho_0 = \frac{1}{Z} e^{-\frac{H_0}{kT}} = \frac{1}{Z} e^{-\beta H_0}$

Operatoren im Gleichgewicht

$$B = B_I = B_H \quad \text{wenn} \quad H = H_0$$

Fall $A = B$

$H_0 |n\rangle = E_n |n\rangle$, $|n\rangle$ vollständig

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

$$A_H(t) = e^{i \frac{H_0 t}{\hbar}} A_S e^{-i \frac{H_0 t}{\hbar}}$$

$$= \frac{i}{\hbar} \frac{\Theta(t - t')}{Z_0} \sum_n \left(\langle n | e^{-\beta H_0} e^{-i \frac{H_0 t}{\hbar}} A_S e^{-i \frac{H_0 t}{\hbar}} e^{-i \frac{H_0 t'}{\hbar}} e^{i \frac{H_0 t'}{\hbar}} A_S e^{i \frac{H_0 t'}{\hbar}} | n \rangle \right)$$

$- \langle r \leftrightarrow r' \rangle$
 $t \leftrightarrow t'$

$\sum_{n'} |n'\rangle \langle n'|$

$$= \frac{i}{\hbar} \frac{\Theta(t - t')}{Z_0} \sum_{n, n'} \langle n | e^{-\beta E_n} e^{-i \frac{E_n t}{\hbar}} A_S(r) e^{-i \frac{E_n t'}{\hbar}} | n' \rangle$$

$$\langle n' | e^{-i \frac{E_{n'} t'}{\hbar}} A_S(r') e^{-i \frac{E_{n'} t}{\hbar}} | n \rangle - \langle r \leftrightarrow r' \rangle$$

$t \leftrightarrow t'$

$$= \frac{i}{\hbar} \frac{\theta(x-x')}{Z_0} \sum \langle m|A(r)|m'\rangle \langle m'|A(r')|m\rangle e^{-\beta E_m} e^{\frac{i}{\hbar} E_m(x-x')} e^{-\frac{i}{\hbar} E_{m'}(x-x')}$$

\sim $r \leftrightarrow r'$
 $t \leftrightarrow t'$

FT $t \rightarrow \omega$

$$\int_0^{\infty} dt e^{i\omega t} e^{-\delta t} = \frac{1}{i\omega + \delta} = i \frac{1}{\omega + i\delta}$$

$$\xrightarrow{\delta \rightarrow 0} i \left(\text{PV} \frac{1}{\omega} - i\pi \delta(\omega) \right)$$

$$\chi(r, r', \omega) = \int_{-\infty}^{\infty} dt \chi(r, r', t) e^{i\omega t}$$

$t = x - x'$

$$= \frac{i}{\hbar} \frac{1}{Z_0} \sum_{m, m'} \langle m|A(r)|m'\rangle \langle m'|A(r')|m\rangle \frac{i e^{-\beta E_m}}{\omega + \frac{E_m - E_{m'}}{\hbar} + i\delta}$$

$$- \langle m|A(r')|m'\rangle \langle m'|A(r)|m\rangle \frac{i e^{-\beta E_m}}{\omega + \frac{E_{m'} - E_m}{\hbar} + i\delta}$$

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

wahl $r = r' \Rightarrow A(r) = A(r') = A$

$$\chi(\omega) = -\frac{1}{\hbar Z_0} \sum_{m, m'} |\langle m|A|m'\rangle|^2 e^{-\beta E_m}$$

$$\left(\frac{1}{\omega + \frac{E_m - E_{m'}}{\hbar} + i\delta} - \frac{1}{\omega - \frac{E_m - E_{m'}}{\hbar} + i\delta} \right)$$

Def. $\chi = \chi' + i\chi''$ $\chi' = \text{Re}(\chi)$ $\chi'' = \text{Im}(\chi)$

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

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

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

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

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

$\langle A(t) A(t') \rangle_0 = \text{Tr}(\rho A(t) A(t'))$ Korrelationsfunktion

$$S(t-t') = \frac{1}{2} \langle A(t) A(t') + A(t') A(t) \rangle_0$$

Symmetrisierte Korrelationsfunktion - Rauschen

$\langle A \rangle = 0$ aber $\begin{matrix} A \\ \uparrow \\ \text{Mittelwert} \end{matrix}$

wie charakterisiert man A ? (das Rauschen)

$\sigma = |t - t'|$ Korrelation klein, wenn

$A(t')$ unabhängig von $A(t)$

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

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

$$\overline{fT} \\ S(\omega) = \frac{1}{Z_0} \sum_{n, m'} |\langle n | A | m' \rangle|^2 e^{-\beta E_n} \left[2\pi \left(\delta\left(\omega + \frac{E_n - E_{m'}}{\hbar}\right) + \delta\left(\omega - \frac{E_n + E_{m'}}{\hbar}\right) \right) \right]$$

$$\int dt e^{i\omega t} = 2\pi \delta(\omega)$$

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

$$S(\omega) = \hbar \coth\left(\frac{\beta \hbar \omega}{2}\right) \chi''(\omega)$$

klassische Limit

$$\coth(x) \approx \frac{1}{x} \quad x \ll 1$$

$$\lim_{\hbar \omega \ll k_B T} \hbar \omega \gg k_B T$$

$$S(\omega) \approx \frac{2}{\omega \beta} \chi''(\omega) = \frac{2k_B T}{\omega} \chi''(\omega)$$

Quantenansatz \longleftrightarrow klass. Ansatz

$$\hbar \omega \geq k_B T$$

$$\hbar \omega \ll k_B T$$

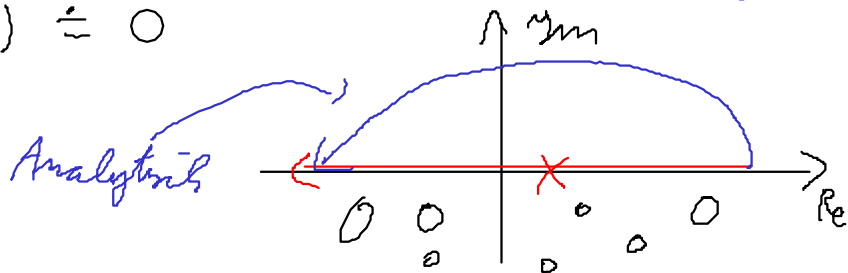
$\chi(t-t') \propto \Theta(t-t') \Rightarrow \chi(\omega)$ Analytisch

für $\text{Im}(\omega) > 0$

$$\chi(\tau) = \int \frac{d\omega}{2\pi} e^{-i\omega\tau} \chi(\omega)$$

$$\omega = i\alpha \Rightarrow e^{\alpha\tau} \\ \tau < 0$$

mit $\chi(\tau < 0) \stackrel{!}{=} 0$



$$\chi'(\omega) = \frac{PV}{\pi} \int d\omega' \frac{\chi''(\omega')}{\omega' - \omega}$$

$$\chi''(\omega) = -\frac{PV}{\pi} \int d\omega' \frac{\chi'(\omega')}{\omega' - \omega}$$

Kramers
Kronig
Relation