Lineare Antwort (Linear Response), Kubo Formel

- Gleichgewicht $\quad W = \rho_0 = \frac{1}{Z} e^{-\frac{H}{kT}}$
- Schwache Anregung $\quad \rho(t) = \rho_0 + \delta\rho \quad\quad \delta\rho \ll$ irgendwas

$\delta\rho$ ist linear in Anregung

Schrödinger Bild

$$i\hbar \dot{\Psi}_S(t) = H(t)\Psi_S(t) \qquad \Psi_S(t) = U(t,t_0)\Psi_S(t_0)$$

$$U(t,t_0) = T \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} H(t')\,dt'\right] \qquad \frac{d}{dt}U(t,t_0) = -\frac{i}{\hbar}H(t)\cdot U(t,t_0)$$

für $H(t) = H_0$: $\quad U(t,t_0) = \exp\left[-\frac{i}{\hbar}H_0(t-t_0)\right]$

Heisenberg Bild

$$O_H(t) = U^+(t,t_0)\,O_S(t)\,U(t,t_0) \qquad \Psi_H = U^+(t,t_0)\Psi_S(t)$$

$$\langle\Psi_H|O_H|\Psi_H\rangle = \langle\Psi_S|O_S|\Psi_S\rangle = \langle\Psi_I|O_I|\Psi_I\rangle$$

$$i\hbar\frac{d}{dt}O_H(t) = [O_H(t), H(t)] + U^+\left(\frac{\partial}{\partial t}O_S\right)U$$

Wechselwirkungs Bild $\hat{=}$ Heisenbergbild mit H_0

$$H = H_0 + V \qquad O_I = \exp\left[\frac{i}{\hbar}H_0 t\right] O_S \exp\left[-\frac{i}{\hbar}H_0 t\right] \qquad t_0 = 0$$

$$\Psi_I(t) = \exp\left[\frac{i}{\hbar}H_0 t\right]\Psi_S(t)$$

$$\begin{aligned}
i\hbar\frac{d}{dt}\Psi_I(t) &= i\hbar H_0 \frac{i}{\hbar}\Psi_I(t) + i\hbar\exp\left[\frac{i}{\hbar}H_0 t\right]\frac{d}{dt}\Psi_S(t)\\
&= -H_0\Psi_I(t) + \exp\left[\frac{i}{\hbar}H_0 t\right](H_0+V)\Psi_S(t)\\
&= -H_0\Psi_I(t) + \exp\left[\frac{i}{\hbar}H_0 t\right](H_0+V)\exp\left[-\frac{i}{\hbar}H_0 t\right]\Psi_I(t)\\
&= V_I(t)\Psi_I(t)
\end{aligned}$$

Dichtematrix $\quad \rho = |\Psi\rangle\langle\Psi|$

$$\rho_I = \exp\left[\frac{i}{\hbar}H_0 t\right]\rho_S\exp\left[-\frac{i}{\hbar}H_0 t\right]$$

$$i\hbar\frac{d}{dt}\rho_I = [V_I, \rho_I]$$

$$\rho_I(t) = \rho_I(t_0) - \frac{i}{\hbar}\int_{t_0}^{t}dt'\,[V_I(t'), \rho_I(t')]$$

- Iteration $\quad \rho(t_0) = \rho_0$

$$\text{①}\quad \rho_I(t) = \rho_0 \underbrace{- \frac{i}{\hbar}\int_{t_0}^{t}dt'\,[V_I(t'), \rho_0]}_{\delta\rho}$$

Beispiel 1

$\hat{A} = \Psi^+(\vec{r})\Psi(\vec{r})$ Dichte

$F = -e\,\varphi(r,t)$ Potential

Beispiel 2

$\hat{A} = \hat{\vec{S}}(\vec{r})$ Magnetisierung

$F = \vec{B}(\vec{r},t)$ Magnetfeld

$$V_S = -\int d^3r\, F(\vec r, t)\, \hat A_S(\vec r)$$

$$\langle B(t)\rangle = \mathrm{Tr}(\rho B) = \mathrm{Tr}(\rho_I(t) B_I(t)) = \overbrace{\mathrm{Tr}(\rho_0 B_I)}^{B_0} \overbrace{- \frac{i}{\hbar}\int_{t_0}^{t} dt'\, \underbrace{\mathrm{Tr}([V_I(t'), \rho_0] B_I(t))}}^{\delta B(\vec r, t)}$$

$$\boxed{\begin{aligned} &= \mathrm{Tr}(V\rho B - \rho V B) \\ &= \mathrm{Tr}(B V \rho - \rho V B) \\ &= \mathrm{Tr}(\rho B V - \rho V B) \\ &= \mathrm{Tr}(\rho [B, V]) \end{aligned}}$$

$$\langle \delta B(\vec r, t)\rangle = -\frac{i}{\hbar}\int_{t}^{t_0} dt'\, \mathrm{Tr}(\rho_0 [B_I(\vec r, t), V_I(t')])$$

$$= \frac{i}{\hbar}\int dt' \int d^3r'\, \mathrm{Tr}(\rho_0 [B_I(\vec r, t), A_I(\vec r', t')])\, F(\vec r', t')$$

$$\delta B(\vec r, t) = \int_{-\infty}^{\infty} dt' \int d^3r'\, \chi_{BA}(\vec r, t, \vec r', t')\, F(\vec r', t')$$

χ Linear-Antwort-Funktion (Response Function)

$$\boxed{\chi(\vec r, t, \vec r', t') = \frac{i}{\hbar}\, \mathrm{Tr}(\rho_0 [B_I(\vec r, t), A_I(\vec r', t')])\, \Theta(t - t')}$$ **Kubo Formel**

- χ ist eine Gleichgewicht-Größe
- homogenes System, Zeit ist homogen $(\vec r, t)$

$\Rightarrow \chi_{BA} = \chi(\vec r - \vec r', t - t')$

$$\boxed{\langle \delta B(\vec k, \omega)\rangle = \chi_{BA}(\vec k, \omega)\, F(\vec k, \omega)}$$

Fluktuations Dissipationstheorem

$\varepsilon(\vec k, \omega)$

$\vec D(\vec k, \omega) = \varepsilon\, \vec E(\vec k, \omega)$

$D = E + 4\pi P$

$$\boxed{-\vec\nabla \vec P = \rho_{el}}$$

$\vec\nabla \equiv i\vec k$

$-ikP = \delta\rho \Rightarrow P = \frac{i\delta\rho}{k}$

$$\boxed{P = \underbrace{-\frac{e\chi_{\rho\rho}}{k^2}}_{\text{Suszeptibilität } \chi} E}$$

für $A = B = \psi^+(r)\psi(r) = \rho_{el}$

$F = -e\varphi(\vec r, t)$

$\delta\rho_{el}(\vec k, \omega) = \chi_{\rho\rho}(\vec k, \omega) \cdot e\,\varphi(\vec k, \omega)$

mit $E = -\nabla\varphi = -ik\varphi$

$P = \frac{i}{k}\delta\rho = \frac{ei}{k}\chi_{\rho\rho}\, i\frac{E}{k}$

$$\boxed{\varepsilon = 1 + 4\pi\chi}$$

Hatle Einschub

$$\boxed{\int_0^\infty e^{-at} = -\frac{1}{a} e^{-at}\Big|_0^\infty = \frac{1}{a}}$$

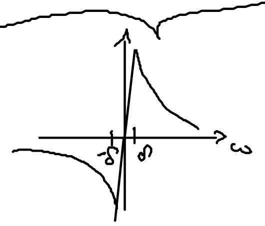
$$\frac{1}{x \mp i\delta} = P\frac{1}{x} \pm \pi\delta(x)$$

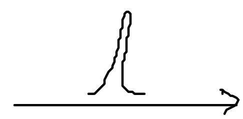
$\delta > 0$ und reell

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

$$\frac{1}{\omega + i\delta} = \frac{\omega - i\delta}{(\omega + i\delta)(\omega - i\delta)} = \frac{\omega - i\delta}{\omega^2 + \delta^2} = \frac{\omega}{\omega^2 + \delta^2} - i\frac{\delta}{\omega^2 + \delta^2}$$

$$\int d\omega \frac{1}{\omega + i\delta} f(\omega) = \int d\omega \frac{\omega}{\omega^2 + \delta^2} f(\omega) - i\int d\omega \overbrace{\frac{\delta}{\omega^2 + \delta^2}}^{\pi\delta(\omega)} f(\omega)$$





$$\lim_{\delta \to 0} \int d\omega \frac{\omega}{\omega^2 + \delta^2} f(\omega) = \text{Prinzipal Value} \int d\omega \frac{1}{\omega} f(\omega)$$