Linear response - Kubo formula

system with small external perturbation

$$\tilde{\mathcal{H}} = \mathcal{H} + \mathcal{H}'(t) = \mathcal{H} + \int d^3r \ \hat{A}(\vec{r}) h(\vec{r}, t) e^{\eta t}$$

adiabatic switching on

$\eta = 0_+$

unperturbed system

coupling to field operators

perturbation

measure: $\langle \hat{B}(\vec{r}, t) \rangle = tr(\hat{\rho}(t) \hat{B}(\vec{r}))$ density matrix $\hat{\rho}(t)$

linear response $\longrightarrow$ $\langle \hat{B}(\vec{r}, t) \rangle = \int dt' \int d^3r' \ \chi_{BA}(\vec{r} - \vec{r}\,', t - t') h(\vec{r}\,', t')$

Kubo formula

$$\chi_{BA}(\vec{r} - \vec{r}\,', t - t') = -\frac{i}{\hbar} \Theta(t - t') \langle [\hat{B}_H(\vec{r}, t), \hat{A}_H(\vec{r}\,', t')] \rangle_{\mathcal{H}}$$

$\hat{A}_H(\vec{r}, t) = e^{i\mathcal{H}t/\hbar} \hat{A}(\vec{r}) e^{-i\mathcal{H}t/\hbar}$ Heisenberg representation

Linear response - Kubo formula

determine density matrix $\hat{\rho}(t)$

equation of motion: $i\hbar\frac{\partial\hat{\rho}}{\partial t} = -[\hat{\rho},\tilde{\mathcal{H}}] = -[\hat{\rho},\mathcal{H}+\mathcal{H}']$

time-dependent perturbation theory

$\hat{\rho} = \hat{\rho}_0 + \delta\hat{\rho}(t)$ with unperturbed (equilibrium) $\hat{\rho}_0 = \frac{1}{Z}e^{-\beta\mathcal{H}}$ $Z = tre^{-\beta\mathcal{H}}$

$$i\hbar\frac{\partial}{\partial t}\delta\hat{\rho} = -[\delta\hat{\rho},\mathcal{H}] - [\hat{\rho}_0,\mathcal{H}'] + \cdots$$

interaction representation

$$\delta\hat{\rho}(t) = e^{-i\mathcal{H}t/\hbar}\hat{y}(t)e^{i\mathcal{H}t/\hbar}$$

$$i\hbar\frac{\partial}{\partial t}\delta\hat{\rho} = -[\delta\hat{\rho},\mathcal{H}] + e^{-i\mathcal{H}t/\hbar}\left\{i\hbar\frac{\partial\hat{y}(t)}{\partial t}\right\}e^{i\mathcal{H}t/\hbar}$$

$\Rightarrow$ $i\hbar\frac{\partial\hat{y}(t)}{\partial t} = -[\hat{\rho}_0,\mathcal{H}'_{int}(t)]$ with $\mathcal{H}'_{int}(t) = e^{i\mathcal{H}t/\hbar}\mathcal{H}'e^{-i\mathcal{H}t/\hbar}$

Linear response - Kubo formula

formal solution: $$\hat{y}(t) = \frac{i}{\hbar}\int_{-\infty}^{t} dt' \; [\hat{\rho}_0, \mathcal{H}'_{int}(t')]$$

$$\langle \hat{B}(\vec{r},t)\rangle = \underbrace{tr\left\{\hat{\rho}_0 \hat{B}(\vec{r})\right\}}_{\substack{0\\ \text{assumption}}} + \underbrace{tr\left\{\delta\hat{\rho}(\vec{r},t)\hat{B}(\vec{r})\right\}}$$

$$tr\left\{\frac{i}{\hbar}e^{-i\mathcal{H}t/\hbar}\int_{-\infty}^{t} dt' \; [\hat{\rho}_0, \mathcal{H}'_{int}(t')]e^{i\mathcal{H}t/\hbar}\hat{B}(\vec{r})\right\}$$

$$\langle \hat{B}(\vec{r},t)\rangle = -\frac{i}{\hbar}\int_{-\infty}^{t} dt' \int d^3r' \; tr\left\{\hat{\rho}_0[\hat{B}_H(\vec{r},t), \hat{A}_H(\vec{r}\,',t')]\right\} h(\vec{r}\,',t')e^{\eta t'}$$

$$= \int dt' \int d^3r' \; \chi_{BA}(\vec{r}-\vec{r}\,', t-t')h(\vec{r}\,',t')$$

Kubo formula

$$\chi_{BA}(\vec{r}-\vec{r}\,', t-t') = -\frac{i}{\hbar}\Theta(t-t')\langle[\hat{B}_H(\vec{r},t), \hat{A}_H(\vec{r}\,',t')]\rangle$$

Linear response - Kubo formula examples

magnetic susceptibility

spin

magnetic field

measure magnetization

perturbation $\mathcal{H}' = -\int d^3r\, \mu_B \hat{S}^z(\vec{r}) h(\vec{r},t)$

$\hat{M}(\vec{r}) = \mu_B \hat{S}^z(\vec{r})$

$$\chi_{zz}(\vec{r}-\vec{r}\,', t-t') = \frac{i}{\hbar}\Theta(t-t')\mu_B^2 \langle [\hat{S}^z_H(\vec{r},t), \hat{S}^z_H(\vec{r}\,',t')]\rangle$$

dielectric susceptibility

charge density

scalar potential

measure charge density

perturbation $\mathcal{H}' = \int d^3r\, e\hat{n}(\vec{r})\phi(\vec{r},t)$

$e\hat{n}(\vec{r})$

$$\chi_e(\vec{r}-\vec{r}\,', t-t') = -\frac{i}{\hbar}\Theta(t-t')e^2 \langle [\hat{n}_H(\vec{r},t), \hat{n}_H(\vec{r}\,',t')]\rangle$$