Quantum Theory of Many-Body systems in Condensed Matter (4302112) 2020

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Today's class: *Linear response theory and Kubo formula*

- Linear response theory.
- Kubo formula.
- Dielectric response.

Linear response theory

Perturbation “turned on” at t_0: $$\hat{H}_t = \hat{H}_0 + \theta(t - t_0)\delta\hat{H}_t$$

“Equilibrium” ($t<t_0$) $$\langle\hat{A}\rangle_0 = \frac{1}{Z_0}\mathrm{Tr}\left[e^{-\beta\hat{H}_0}\hat{A}\right]$$

“Non-Equilibrium” ($t>t_0$) $$\langle\hat{A}\rangle(t) = \langle\hat{A}\rangle_0 + \delta\langle\hat{A}\rangle(t)$$

To first order (Kubo formula):

[redacted] $$\langle\hat{A}\rangle(t) \approx \langle\hat{A}\rangle_0 - i\int_{t_0}^{t} dt_1 \left\langle \left[\hat{A}_I(t), (\delta\hat{H}_t)_I(t_1)\right]_- \right\rangle_0 .$$

$$\hat{A}_I(t) \equiv e^{+i\hat{H}_0 t}\hat{A}e^{-i\hat{H}_0 t} \qquad (\delta\hat{H}_t)_I(t) \equiv e^{+i\hat{H}_0 t}\delta\hat{H}_t e^{-i\hat{H}_0 t}$$

Kubo formula in frequency domain

Alternatively: $$\delta\langle\hat{A}\rangle(t) \approx \int_{t_0}^{\infty} dt_1\, C^R_{\hat{A},\delta\hat{H}_t}(t,t_1)\ .$$

with $$C^R_{\hat{A},\hat{H}'_t}(t,t_1) = -i\theta(t-t_1)\left\langle \left[\hat{A}_I(t),(\delta\hat{H}_t)_I(t_1)\right]_- \right\rangle_0\ .$$

Retarded correlation function

If $\delta\hat{H}_t = \hat{B}f(t)$ in *frequency* domain: ⇒ $\delta\langle\hat{A}\rangle(\omega^+) = C^R_{\hat{A},\hat{B}}(\omega^+)f(\omega^+)$

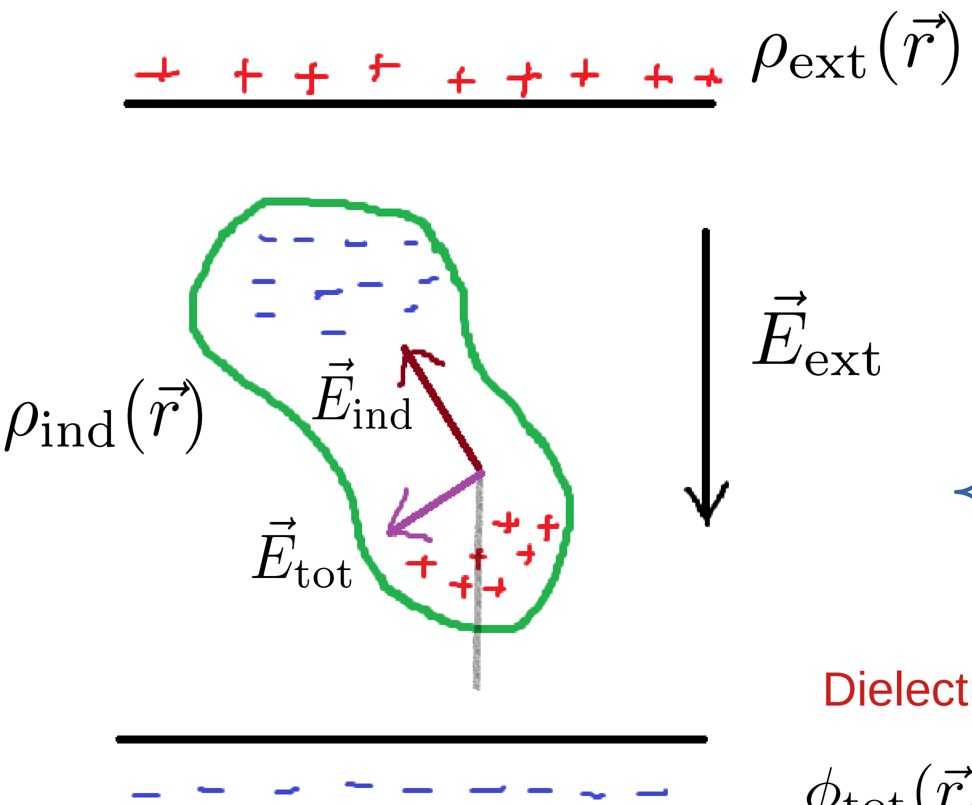
- Special case: $\delta\hat{H}_t = \hat{A}f(t)$

$$\langle\hat{A}\rangle(\omega^+) = \langle\hat{A}\rangle_0 + \chi^R_{\hat{A}}(\omega)f(\omega^+)$$

"Dynamical Susceptibility"

$\hat{A}$	$\chi^R_{\hat{A}}(\omega)$
charge density	charge susceptibility
spin density	spin susceptibility
current density	Current-current correlation function

Example: Dielectric response



$$\rho_{\mathrm{ind}}(\vec{r}) = \rho(\vec{r}, t > t_0) - \rho_0(\vec{r})$$

$$\vec{E}_{\mathrm{tot}} = \vec{E}_{\mathrm{ext}} + \vec{E}_{\mathrm{ind}}$$

$$\vec{E} = \vec{D}/\epsilon_0 - \vec{P}/\epsilon_0 \Rightarrow \vec{D} = \epsilon_0 \vec{E} + \vec{P}$$

$$\begin{cases} \rho_{\mathrm{tot}} = \rho_{\mathrm{ext}} + \rho_{\mathrm{ind}} \\ \phi_{\mathrm{tot}} = \phi_{\mathrm{ext}} + \phi_{\mathrm{ind}} \end{cases} \qquad \nabla^2 \phi_{(\dots)} = -\rho_{(\dots)}/\epsilon_0$$

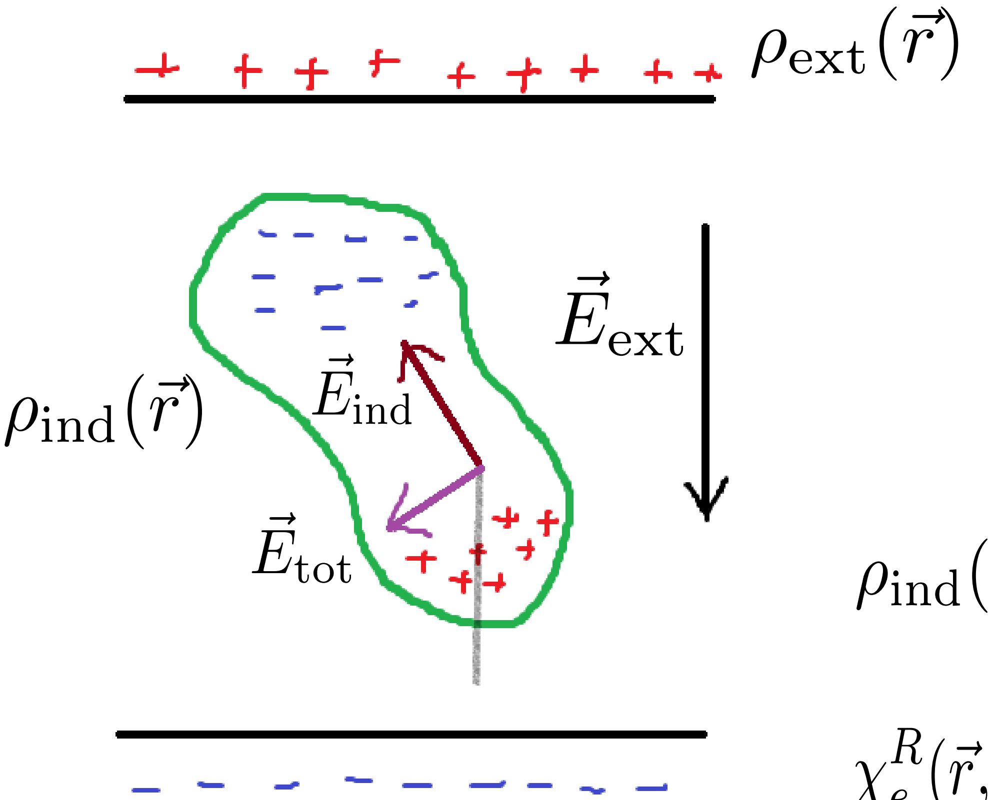
Dielectric function:

$$\phi_{\mathrm{tot}}(\vec{r}, t) = \int d\vec{r}_1 dt_1 \; \epsilon^{-1}(\vec{r}, t; \vec{r}_1, t_1) \phi_{\mathrm{ext}}(\vec{r}_1, t_1)$$

Isotropic, linear case:

$$\vec{D} = \frac{\epsilon_0}{\epsilon^{-1}} \vec{E} \equiv \epsilon \epsilon_0 \vec{E}$$

Perturbative quantum limit



$$\rho_{\text{ind}}(\vec{r}) = \langle \hat{\rho}_e(\vec{r}) \rangle(t) - \langle \hat{\rho}_e(\vec{r}) \rangle_0$$

$$\hat{\rho}_e(\vec{r}) = -e\hat{\psi}^\dagger(\vec{r})\hat{\psi}(\vec{r})$$

Perturbation (external potential):

$$\delta \hat{H}_t = \int d\vec{r}\; \hat{\rho}_e(\vec{r})\phi_{\text{ext}}(\vec{r}, t)$$

$$\rho_{\text{ind}}(\vec{r}, t) = \int d\vec{r}_1 dt_1\; \chi_e^R(\vec{r}t; \vec{r}_1 t_1)\phi_{\text{ext}}(\vec{r}_1, t_1)$$

$$\chi_e^R(\vec{r}, t; \vec{r}_1, t_1) = -i\theta(t - t_1)\left\langle [\hat{\rho}_e(\vec{r}, t), \hat{\rho}_e(\vec{r}_1, t_1)]_- \right\rangle_0$$

Density-density correlation function (“Polarizability”)

Dielectric response (linear)

$$\nabla^2 \phi_{\rm ind}(\vec{r}) = -\frac{\rho_{\rm ind}(\vec{r},t)}{\epsilon_0} \Rightarrow \phi_{\rm ind}(\vec{r},t) = \int d\vec{r}_1 \; U(\vec{r}-\vec{r}_1)\rho_{\rm ind}(\vec{r}_1,t)$$

Coulomb potential

$$\epsilon^{-1}(\vec{r},t;\vec{r}_1,t_1) = \delta(\vec{r}-\vec{r}_1)\delta(t-t_1) + \int d\vec{r}_2 \, U(\vec{r}-\vec{r}_2)\chi_e^R(\vec{r}_2 t;\vec{r}_1 t_1)$$

Fourier transform (translation invariant systems!)

$$\epsilon^{-1}(\vec{q},\omega) = 1 + U(\vec{q})\chi_e^R(\vec{q},\omega)$$

Dielectric response

with

$$U(\vec{q}) = \int d\vec{r} \, e^{i\vec{q}\cdot\vec{r}} \frac{e^2}{4\pi\epsilon_0 r} = \frac{e^2}{\epsilon_0 q^2}$$

$$\chi_e^R(\vec{q},\omega) = \int d(t-t') \int d(\vec{r}-\vec{r}\,') \, e^{-i\vec{q}\cdot(\vec{r}-\vec{r}\,')} e^{+i\omega^+(t-t')} \chi_e^R(\vec{r}-\vec{r}\,',t-t')$$