2 Green's functions

2.1 Response functions

2.1.1 Experimental techniques

There are three broad categories of experimental probes in condensed matter physics:

- thermodynamics
- transport
- spectroscopy

Thermodynamics can be computed by differentiating the partition function Z with respect to a few global variables (temperature, magnetic field, pressure, ...)

$\longrightarrow$ highly universal $\oplus$

$\longrightarrow$ no information about spatial & dynamical structure $\ominus$

$\Rightarrow$ thermodynamics alone insufficient to investigate microscopic properties of a system.

Transport and Spectroscopy techniques:

- use electromagnetic forces as external perturbation
  - photons (optics, x-rays, photoemission)
  - voltage drop (transport)
  - spin magnetic moments (e.g., neutron scattering)
- response of the system (emitted/scattered particles) probed by a detector

Formalism: Linear-response theory

2.1.2 Linear-response theory

Experiment: switch on a small field $\delta h(\vec{r},t)$

Linear response: small deviations from thermal equilibrium

Assumptions: minimal coupling of δh to system observable $A(\vec{r})$:

$$\boxed{\begin{aligned} H(t) &= H_0 + H_1(t) \\ H_1(t) &= -\int d^3r\, \delta h(\vec{r},t)\, A(\vec{r}) \end{aligned}}$$

[here written as "scalar • scalar" coupling, can be generalized to "vector • vector"]

Examples:
- $A \to \vec{S}$ (spin), $\delta h \to \mu_B \delta\vec{H}$ (magnetic field) $\to$ magnetic susceptibility $\chi(\vec{q},\omega)$
- $A \to \vec{j}$ (current density), $\delta h \to \frac{e}{c}\delta\vec{A}$ (vector potential) $\Rightarrow$ optical conductivity $\overleftrightarrow{\sigma}(\omega)$

Strategy: Linear response from time-dependent perturbation theory

Question: how does an observable $\langle B(\vec{r},t)\rangle$ change due to external perturbation $\delta h(\vec{r},t)$ that couples to $A(\vec{r},t)$?

$$\boxed{\langle B(\vec{r},t)\rangle = \langle \vec{B}(\vec{r})\rangle_{eq} + \underbrace{\delta\langle B(\vec{r},t)\rangle}_{\text{"small" in a sense specified below}}}$$

For $t \to -\infty$ the system is in thermal equilibrium

Schrödinger picture: $\langle B(\vec{r},t)\rangle = \mathrm{Tr}\big[\underbrace{\rho(t)}_{\text{density matrix}}\, B(\vec{r})\big]$; $\mathrm{Tr}[\rho(t)] = 1$

(1) Density matrix solves von Neumann equation

$$\boxed{i\hbar\,\partial_t \rho(t) = [H(t), \rho(t)]} \quad (*)$$

with initial condition $\rho(t\to-\infty) = \rho_0$, $[H_0, \rho_0] = 0$.

Canonical ensemble: $\rho_0 = \dfrac{e^{-\beta H_0}}{\mathrm{Tr}\, e^{-\beta H_0}}$

Linear response: $\rho(t) = \rho_0 + \overbrace{\delta\rho(t)}^{\text{deviation from equilibrium linear in } \delta h}$

with $\boxed{i\hbar\,\partial_t \rho(t) = [H_0, \delta\rho(t)] + [H_1(t), \rho_0] + \mathcal{O}(\delta h^2)}$

Solution: $\delta\rho(t) = \frac{1}{i\hbar}\int_{-\infty}^{t} d\tau\; e^{-iH_0(t-\tau)/\hbar}\,[H_1(\tau), \rho_0]\,e^{iH_0(t-\tau)/\hbar}$ from (*)

(**)

check: $\partial_t\,\delta\rho(t) = \frac{1}{i\hbar}\, e^{-iH_0(t-t)/\hbar}\,[H_1(t), \rho_0]\,e^{iH_0(t-t)/\hbar}$

$- \frac{i}{\hbar} H_0\,\delta\rho(t) + \frac{i}{\hbar}\,\delta\rho(t)\,H_0$ ✓

② use linear-in-δh solution for $\delta\rho(t)$ to compute linear-in-δh response for system observable B:

$$\langle B(\vec r, t)\rangle = \mathrm{Tr}[\rho_0 B(\vec r)] + \mathrm{Tr}[\delta\rho(t)\, B(\vec r)]$$

$$\delta\langle B(\vec r, t)\rangle = \mathrm{Tr}[\delta\rho(t)\, B(\vec r)] \overset{(**)}{=}$$

$$= - \frac{1}{i\hbar}\int_{-\infty}^{t} d\tau \int d^3r'\; \mathrm{Tr}\Big[\big[\underbrace{e^{iH_0\tau/\hbar} A(\vec r\,') e^{-iH_0\tau/\hbar}}_{A(\vec r\,', \tau)\text{ interaction picture}}, \rho_0\big] \times$$

from $H_1 = -\int A\,\delta h$

$$\times \underbrace{\big[e^{iH_0 t/\hbar} B(\vec r) e^{-iH_0 t/\hbar}\big]}_{B(\vec r, t)} \times$$

$$\times\; \delta h(\vec r\,', \tau) = \ldots$$

use $\mathrm{Tr}\,[[a,b]\,c] = \mathrm{Tr}\,([c,a]\,b)$, set $t' = \tau$

$$\ldots = \frac{i}{\hbar}\int_{-\infty}^{t} dt' \int d^3r'\; \underbrace{\mathrm{Tr}\big[[B(\vec r, t), A(\vec r\,', t')]\,\rho_0\big]}_{\langle [B,A]\rangle_{eq}}\; \delta h(\vec r\,', t')$$

Result: $\boxed{\delta\langle B(\vec r, t)\rangle = \frac{i}{\hbar}\int_{-\infty}^{t} dt' \int d^3r'\; \langle [B(\vec r, t), A(\vec r\,', t')]\rangle_{eq}\; \delta h(\vec r\,', t')}$

Remarks: (i) convolution in real space & time $(\vec{r},t)$

$\Rightarrow$ product in Fourier space $(\vec{q},\omega)$

(ii) the linear response function is thus defined as the retarded commutator

$$\boxed{\chi^R_{BA}(\vec{r},t;\vec{r}',t') \equiv \frac{i}{\hbar}\underbrace{\langle[B(\vec{r},t),A(\vec{r}',t')]\rangle_{eq}}_{\text{commutation}}\underbrace{\Theta(t-t')}_{\text{retardation}}}$$

(iii) if the equilibrium state is spatially and temporally translationally invariant:

$$\chi^R_{BA}(\vec{r},t;\vec{r}',t') \equiv \chi^R_{BA}(\vec{r}-\vec{r}',t-t')$$

$$\xRightarrow{\text{Fourier}} \boxed{\delta\langle B(\vec{q},\omega)\rangle = \chi^R_{BA}(\vec{q},\omega)\,\delta h(\vec{q},\omega)}$$

with $\chi^R_{BA}(\vec{q},\omega) = \lim_{\eta\to 0^+}\int_{-\infty}^{\infty}dt\int d^3r\, e^{i\vec{q}\vec{r}}\, e^{-i(\omega+i\eta)t}\,\chi^R_{BA}(\vec{r},t)$

- $\eta \to$ convergence factor ensuring causality (poles of χ are in lower half complex plane; $\sim \frac{1}{\omega-E+i0^+} \Rightarrow$ poles at $\omega = \underset{\substack{\text{real}\\\text{excitation}\\\text{energy}}}{E} - i0^+$)
- $e^{-i\cdot i\eta t} = e^{\eta t}$ can also be understood as "adiabatic switching on" of perturbation as $t\to-\infty$.

(iv) the retarded commutator is a Green's function

$$\chi^R_{BA}(\ldots) \equiv G^R_{BA}(\ldots)$$

in most cases a "two-particle Green's function" $\to$ e.g. density-density, spin-spin response

$\to$ later we will also encounter the one-particle Green's fct.

(a) Properties of the response function

Observables A and $\mathbb{B}$ are hermitean operators; therefore (using G instead of χ for real space and time)

$$\boxed{G^R_{BA} \text{ is real}}$$

$$G^{R\,*}_{BA} = -\frac{i}{\hbar}\langle \underbrace{[B,A]^+}_{[A^+,B^+]=-[B,A]} \rangle_{eq}\,\Theta(t-t') = \frac{i}{\hbar}\langle [B,A]\rangle_{eq}\,\Theta(t-t') = G^R_{BA} \checkmark$$

For $\chi_{BA}(\vec{q},\omega) = \chi'_{BA} + i\chi''_{BA}$ it follows that (suppressing $\vec{q}$)

$$\boxed{\begin{array}{lll} \chi'_{BA}(-\omega) = \chi'_{BA}(\omega) & & \text{real part even} \\ \chi''_{BA}(-\omega) = -\chi''_{BA}(\omega) & & \text{imag. part odd} \end{array}}$$

(b) Causality

The step function $\Theta(t-t')$ in $G^R_{BA}(t-t')$ is a consequence of causality: $B(t)$ can only be influenced by an earlier $\delta h(t')$, i.e., for $t \geq t'$.

(c) Lehmann representation

Assume that we know the exact eigenstates of H_0:

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

The statistical operator for the canonical ensemble is

$$\frac{e^{-\beta H_0}}{Z} \Rightarrow \frac{e^{-\beta E_n}}{Z}, \quad Z = \operatorname{tr} e^{-\beta H_0} = \sum_n e^{-\beta E_n}$$

$$\Rightarrow G^R_{BA}(t) = \frac{i}{\hbar}\Theta(t)\frac{1}{Z}\sum_{nn'} e^{-\beta E_n}\Big[\langle n|e^{iH_0t/\hbar}Ae^{-iH_0t/\hbar}|n'\rangle\langle n'|B|n\rangle -$$

$$-\langle n|B|n'\rangle\langle n'|e^{iH_0t/\hbar}Ae^{-iH_0t/\hbar}|n\rangle\Big] = \ldots$$

$$= \frac{i}{\hbar}\,\Theta(t)\,\frac{1}{Z}\sum_{nn'} e^{-\beta E_n}\Big[e^{i(E_n-E_{n'})t/\hbar}\langle n|A|n'\rangle\langle n'|B|n\rangle$$
$$- e^{-i(E_n-E_{n'})t/\hbar}\langle n|B|n'\rangle\langle n'|A|n\rangle\Big].$$

The Laplace transform $\int_0^\infty dt\, e^{i(\omega+i\eta)t}\, G^R_{AB}(t) \equiv \chi_{AB}(\omega+i\eta)$

yields, because of $\frac{i}{\hbar}\int_0^\infty dt\, e^{i(\omega+i\eta)t}\, e^{\pm i(E_n-E_{n'})t/\hbar}$

$$= -\frac{1}{\hbar(\omega+i\eta)\pm(E_n-E_{n'})}$$

the relation

$$\boxed{\chi^R_{AB}(\omega+i0^+) = -\frac{1}{Z}\sum_{nn'} e^{-\beta E_{n'}}\left[\frac{\langle n|A|n'\rangle\langle n'|B|n\rangle}{\hbar\omega+E_n-E_{n'}+i0^+} - \frac{\langle n|B|n'\rangle\langle n'|A|n\rangle}{\hbar\omega-E_n+E_{n'}+i0^+}\right]}$$

Lehmann representation.

In the thermodynamic limit the complex response function has a close sequence of poles slightly below the real axis at $\hbar\omega = \pm(E_n-E_{n'}) - i0^+$.

The imaginary part is given via the Dirac relation

$$\frac{1}{\omega+i0^+} = \underbrace{\mathcal{P}\frac{1}{\omega}}_{\substack{\text{principal}\\ \text{value under}\\ \text{the integral}}} - i\pi\,\delta(\omega)$$

by $$\chi''_{AB}(\omega) = \pi \frac{1}{Z} \sum_{nn'} e^{-\beta E_n} \Big[\delta(\hbar\omega + E_n - E_{n'}) \langle n|A|n'\rangle \langle n'|B|n\rangle$$
$$- \underbrace{\delta(\hbar\omega - E_n + E_{n'}) \langle n|B|n'\rangle \langle n'|A|n\rangle}_{\text{rename } n \leftrightarrow n'} \Big]$$

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

Most important case: $A = B$

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

Fermi's golden rule

$$\chi'_{AA}(\omega) = -\frac{1}{Z} \sum_{nn'} \mathcal{P} \frac{|\langle n|A|n'\rangle|^2}{\hbar\omega + E_n - E_{n'}} \left(e^{-\beta E_n} - e^{-\beta E_{n'}}\right).$$

Some properties of response functions:

(i) Selection rules: matrix elements $\langle n|A|n'\rangle$ "select" states that are connected by the A-operator. $\Rightarrow$ choose a probing technique with A to learn about the states of interest.

(ii) high-frequency limit $\lim_{\omega\to\infty} \chi'_{AA}(\omega) \sim \frac{1}{\omega^2}$

(iii) Energy dissipation: can show that $\omega\chi''_{AA}(\omega) \geq 0$
$\Rightarrow$ energy transferred to the system is ≥ 0.

(iv) Kramers-Kronig relations:

$$\chi'_{A}(\omega) = -\frac{1}{\pi} \mathcal{P} \int d\omega' \frac{\chi''_{AA}(\omega')}{\omega - \omega'}$$
$$\chi''_{A}(\omega) = \frac{1}{\pi} \mathcal{P} \int d\omega' \frac{\chi'_{AA}(\omega')}{\omega - \omega'}$$

Skipped for this lecture: fluctuation-dissipation theorem.
(but important)