Transport: Basics.

I. The Kubo formula

Recall basics from linear response theory:

$$\left.\begin{aligned}\hat{H}(t) &= \hat{H}_0 - a(t)\hat{A} \\ \hat{\rho}(t) &= \hat{\rho}_0 + \delta\hat{\rho}(t)\end{aligned}\right\} \Rightarrow \delta\hat{\rho}(t) = \frac{i}{\hbar}\int_{-\infty}^{t} dt'\, a(t') \left[\underbrace{A^{(I)}(t'-t)}_{\downarrow}, \hat{\rho}_0 \right]$$

(Recall interaction representation: $\hat{A}^{(I)}(t'') = e^{iH_0t''}\hat{A}\, e^{-iH_0t''}$)

Then $\langle \hat{B}(t)\rangle_a = \mathrm{Tr}(\hat{\rho}(t)\hat{B}) = \int_{-\infty}^{+\infty} \tilde{\chi}_{BA}(t-t')\, a(t')\, dt'$

susceptibility.

where:

Kubo formula: $\left[\tilde{\chi}_{BA}(t) = \frac{i}{\hbar}\Theta(t) \langle [B(t), A] \rangle_0 \right]$ $\leftarrow$ $\mathrm{Tr}(\hat{\rho}_0 \cdot)$

$$\left.\begin{aligned}\hat{\rho}_0 &= e^{-i\beta\hat{H}_0} \\ i\hbar\dot{\hat{A}} &= [A, H_0]\end{aligned}\right\} \longrightarrow \;= \beta\,\Theta(t)\, \tilde{K}_{B\dot{A}}(t)$$

@ this order

response kernel

$$= \frac{1}{\beta}\int_0^\beta \langle \dot{A}(-i\hbar\lambda)\, B(t)\rangle_0\, d\lambda$$

$\uparrow$

this latter version is the "Green-Kubo formula".

$\rightarrow$ response function $\hat{=}$ correlations

(cf also fluctuation-dissipation etc)

$\Longrightarrow$ if $\begin{aligned} B &= \text{current} \\ A &= \text{density}\end{aligned}$ then χ is a current-current correlation.

II. Two applications

1) The Onsager relations

$$J_i(\vec{r},t) = \sum_j L_{ij}\, \underbrace{F_j(\vec{r},t)}_{\text{"generalized force" (intensive)}}$$

→ conjugate extensive variable: $X_j(\vec{r},t)$.

"Conjugate" $\leftrightarrow$ "Equipartition": $\langle \delta X_i\, F_j \rangle = -k_B\, \delta_{ij}$

First assumption: $\langle \delta X_i\, \delta X_j(\tau)\rangle = \langle \delta X_i(\tau)\, \delta X_j\rangle$

(time-translation + time reversal) ↳ (improved by Casimir)

Then $\langle \delta X_i\, \underbrace{\delta \dot{X}_j}_{= \sum_k L_{jk} F_k} \rangle = \langle \underbrace{\delta \dot{X}_i}_{= \sum_k L_{ik} F_k}\, \delta X_j \rangle$

that's Onsager's "regression hypothesis"

which implies: $\boxed{L_{ij} = L_{ji}}$ → Onsager relations.

NB: in particular, no Hall effect when TR is not broken.

2) The Kubo-Nakano formula

That's a special case of Green-Kubo with electronic transport.

$\hat{H}_1(t) = -e\sum_i \hat{r}_{i,\beta}\, E_\beta(t)$ and the response is $\hat{B} = \hat{J}_\alpha$, the charge current.

thus

$\hat{A} = e\sum_i \hat{r}_{i\beta}$

$a(t) = -E_\beta(t)$

$$\boxed{\begin{aligned} &\Rightarrow \tilde{\chi}_{BA}(t) = \Theta(t)\int_0^\beta \langle J_\beta(-i\hbar\lambda)\, J_\alpha(t)\rangle\, d\lambda \\ &\text{and by def, } \sigma_{\alpha\beta}(\omega) = \int_0^\infty dt\, e^{i\omega t}\, \tilde{\chi}_{BA}(t). \end{aligned}}$$

Kubo-Nakano formula for σ.

III. The London approach

$$H = \int d^3\vec{x} \left\{ \frac{1}{2m} \psi^\dagger(x) \left(-i\hbar\vec{\nabla} - e\vec{A}\right)^2 \psi(\vec{x}) - e\,\phi(\vec{x})\,\psi^\dagger(\vec{x})\psi(\vec{x}) \right\}.$$

$$\Rightarrow \vec{J}(\vec{x}) = -\frac{\delta H}{\delta \vec{A}(\vec{x})} = \underbrace{\frac{-ie\hbar}{2m} \psi^\dagger \overleftrightarrow{\nabla} \psi(\vec{x})}_{= \vec{J}_P \text{ "paramagnetic"}} + \underbrace{\frac{-e^2}{m} \vec{A}(\vec{x})\,\rho(x)}_{= \vec{J}_D \text{ "diamagnetic"}}$$

Rq: decomposition not gauge-invariant under $\left| \begin{array}{l} \psi(\vec{x}) \to e^{ie\chi(\vec{x})}\psi(\vec{x}) \\ A(\vec{x}) \to \vec{A}(\vec{x}) + \hbar\vec{\nabla}\chi(\vec{x}) \end{array} \right.$

Apply linear response with $H_1 = -\int d^3x\, \vec{J}_P(x)\, \vec{A}(x)$ minimal coupling.

This yields: (only this one is not trivial)

$$\langle j_P^\alpha(t) \rangle = \int_{t'<t} dt'\, d^3\vec{x}'\; i \left\langle \left[j_P^\alpha(x), j_P^\beta(x') \right] \right\rangle A^\beta(x')$$

the London response kernel

$$\Rightarrow \vec{J}(1) = -\int d2\; \underline{Q}(1-2)\, \vec{A}(2)$$

(same here)

where

$$\boxed{Q^{\alpha\beta}(1-2) = \underbrace{\frac{ne^2}{m} \delta^{\alpha\beta} \delta(1-2)}_{\text{"diamagnetic response"}} - \underbrace{i \left\langle \left[j_P^\alpha(1), j_P^\beta(2) \right] \right\rangle \theta(t_1 - t_2)}_{\text{"paramagnetic response"}}}$$

Now conductivity:

$$\left. \begin{array}{l} \sigma^{\alpha\beta} = \dfrac{1}{-i\nu} Q^{\alpha\beta} \\ Q(\nu = 0) \stackrel{!}{=} 0 \end{array} \right\} \Rightarrow \boxed{\sigma^{\alpha\beta}(\nu) = \frac{1}{-i\nu} \left(-i \langle j^\alpha(\omega)\, j^\beta(-\omega) \rangle \right) \Big|_{\omega=0}^{\omega=\nu}}$$

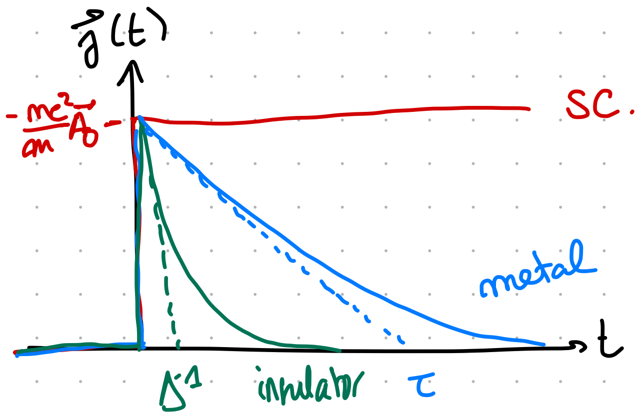
Kubo-Nakano recovered!

<u>Interpretation:</u> take $\vec{A}(t) = \vec{A}_0\,\Theta(t)$

and free bulk electrons, $m\dfrac{d\vec{v}}{dt} = -e\left(-\dfrac{d\vec{A}}{dt}\right)$.

One gets $\vec{j}_P = \vec{0}$ and $\vec{j}_D = -\dfrac{ne^2}{m}\vec{A}_0$: a pure "diamagnet" : a superconductor.

More generally :



At $t=0^+$, every material "is a SC".
(that's the f-sum rule, see P. Coleman's book).

So: $\vec{j}_D$ is the "superconducting" response.
$\vec{j}_P$ comes later to balance it.

Two very different behaviours :

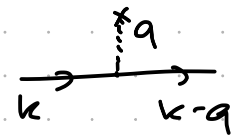
- $\vec{j} \propto \vec{A}$: in SC, plasma, metal @ high ω.
  ↳ a "Higgsed" phase, KG equation, diamagnetic.
- $\vec{j} \propto \dfrac{d\vec{A}}{dt}$: in a metal @ low ω, dielectrics.
  ↳ a "Coulomb" phase, mostly paramagnetic.

→ Now how does one actually compute the London kernel?

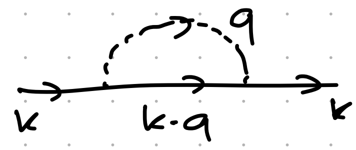
IV. A hint of diagrams.

1) Electron scattering on disorder

$$\hat{V} = \int d^3x \, \underbrace{U(x)}_{\text{white noise}} \psi^\dagger(x)\psi(x)$$

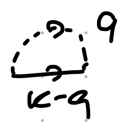


Basic block after averaging over the disorder:



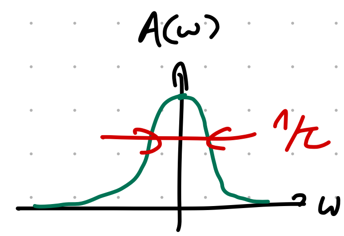
$$\Rightarrow \; G(k, i\omega_m) = \frac{1}{i\omega_m - \epsilon_k - \Sigma(i\omega_m)}$$

$(\tau = \pi n_i u_0^2)$

where $\Sigma(i\omega_m) \simeq \int dq$  $= n_i \sum_{k'} \frac{|u(k-k')|^2}{i\omega_m - \epsilon_{k'}} = -\frac{i}{2\tau} \,\mathrm{sign}(\omega_m)$.

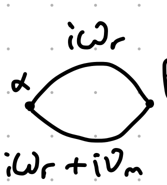
$$\Rightarrow G(k, z) = \left[z - \epsilon_k + \frac{i}{2\tau}\,\mathrm{sign}(\mathrm{Im}\, z)\right]^{-1}$$

Spectral function: $A(k, \omega) = \frac{1}{\pi}\,\mathrm{Im}\, G(k, \omega - i\delta) =$



2) Drude conductivity.

The current vertex is $\alpha \langle \; \equiv \frac{e k^\alpha}{m}$. Response kernel?

$\langle j^\alpha(i\nu_m) j^\beta(-i\nu_m)\rangle =$  $= -2T \sum_{k, i\omega_r} \frac{k^\alpha k^\beta}{m^2} e^2 G(k, i\omega_r + i\nu_m) G(k, i\omega_r)$

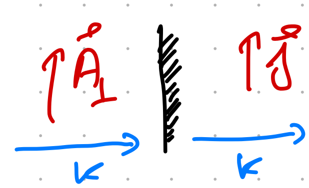
Matsubara sum: see textbook. Result: $\boxed{\sigma^{\alpha\beta}(\nu + i\delta) = \frac{ne^2}{m} \frac{1}{-i\nu + \tau^{-1}}}$.

Drude.

⚠ Rk: this is all about transverse conductivity.

i.e. $\partial_t \rho = -\mathrm{div}\, \vec{j} = 0$

i.e. "fast response" $\neq$ diffusive (see later).



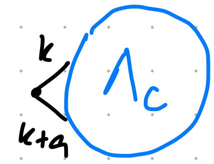
V. Electronic diffusion.

Now we are considering the other case: $\partial_t \rho = -\mathrm{div}\,\vec{j} \neq 0.$

↳ Apply $\phi(q) \to$ response $\delta\rho(q)$. "slow response"

$$\langle \delta\rho(q) \rangle \overset{\text{kubo}}{=} i \underbrace{\langle [\rho(q, i\nu_m), \rho(-q, -i\nu_m)] \rangle}\,(-e\phi(q))$$

$$= -2T\, G(k+q)\, G(k) .\ \Lambda_c(k, k+q) .$$



Random phase approximation: $\langle [\rho, \rho] \rangle =$ 

$$\Lambda_c(k, k+q) = (\text{see P. Coleman}) = \frac{\tau^{-1}}{\nu_m + Dq^2} \qquad (D = v_F^2/3).$$

$$\Rightarrow \boxed{\chi(q, \nu + i\delta) = \chi_0 \frac{Dq^2}{Dq^2 - i\nu}} \longleftarrow \text{diffusive pole} \neq \text{Drude !}$$

$$\left.\begin{array}{l} \delta\rho(q) = \chi(q)\, e\,\phi(q) \\ -i\vec{q}\,\vec{j}(q) = e\dot{\rho} = -i\nu\,\delta\rho(q) \end{array}\right\} \xrightarrow[\vec{j}(q) = \sigma_L(q)\vec{E}(q)]{q^2\phi(q) = i\vec{q}\vec{E}(q)} \boxed{\sigma_L(q) = e^2\chi_0 D \frac{i\nu}{i\nu - Dq^2}}$$

Einstein's relation.

[☺ NB: $\sigma_L(q)$ is transverse (i.e. fast) while $\chi(q)$ is diffusive (i.e. slow)
but they're the same thing ultimately!]

Cf Luttinger '64 version: $\phi_q(t) = \phi_q e^{st}$, $s \to 0$.

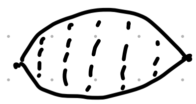
$$\left\{\begin{array}{l} \dot{\rho}(r) + \vec{\nabla}\vec{j}(r) = 0 \\ j_\alpha(r) = \sigma_{\alpha\beta} E_\beta(r) - D_{\alpha\beta} \nabla_\beta \rho(r) \end{array}\right\} \leftrightarrow \left\{\begin{array}{l} \langle \rho_q \rangle = -\dfrac{\vec{q}\,\underline{\sigma}\,\vec{q}}{s + \vec{q}\,\underline{D}\,\vec{q}}\,\phi_q \\ \langle j^\alpha_q \rangle = \left(\sigma_{\alpha\beta} - D_{\alpha\beta} \dfrac{\vec{q}\,\underline{\sigma}\,\vec{q}}{s + \vec{q}\,\underline{D}\,\vec{q}}\right) E_\beta(q) \end{array}\right.$$

both here!

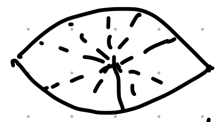
- Rapid: $\lim_{s\to 0} \lim_{q \to 0}$: then $\langle \rho_q \rangle = 0$, $\langle \vec{j}_q \rangle = \underline{\sigma}\,\vec{E}_q$: transverse.
- Slow: $\lim_{q\to 0} \lim_{s \to 0}$: then $\langle \vec{j}_q \rangle = \vec{0}$ and $\left[\sigma_{\alpha\beta} = \dfrac{\vec{q}\,\underline{\sigma}\,\vec{q}}{\vec{q}\,\underline{D}\,\vec{q}} D_{\alpha\beta} \right]$ (diffusion) Einstein's relation again.

VI. Two remarks.

1) Other diagrams are sometimes important.

Recall that to get Drude we summed diagrams like .

$\rightsquigarrow$ incoherent scattering time $\tau \sim \ell/\sqrt{D}$.

But $\exists$ "Langer-Neal" diagrams:  (cf mesoscopic physics etc).

$\rightsquigarrow$ coherent scattering time $\tau_0 \sim L/\sqrt{D}$

$$\Rightarrow \text{Correction } \Delta\sigma \propto \int_{(D\tau_0)^{-1/2}}^{(D\tau)^{-1/2}} \frac{d^dq}{(2\pi)^d} \frac{1}{Dq^2 - i\nu} \overset{d=2}{=} -\frac{1}{2\pi^2}\frac{e^2}{\hbar} \ln(\tau_0/\tau).$$

$\rightarrow$ For $\underline{L = \ell e^{2\pi k_F \ell}}$ one gets $\underline{\sigma_{tot} = \sigma_{Drude} + \Delta\sigma = 0}$.

$\hookrightarrow$ nonperturbative wrt disorder (usual result of RG).

Anderson localization

2) Thermal conductivity?

$$\left\{\begin{array}{l} \vec{J} = \underline{\underline{\sigma}}\vec{E} = -\sigma\vec{\nabla}\phi \\ \partial_t \rho_e + \operatorname{div}\vec{J}_e = 0 \end{array}\right\} \overset{?}{\longleftrightarrow} \left\{\begin{array}{l} \vec{J} = -K\vec{\nabla}T \\ \partial_t h_Q + \operatorname{div}\vec{J}_Q = 0 \end{array}\right\}$$

Problem: T is not an external potential. No minimal coupling!

So the transverse viewpoint (i.e. fast response) is fishy.

However, $H_1 = -e\int \rho_e(r)\phi(r)\,d\vec{r} \overset{\text{OK}}{\Leftrightarrow} H_1 = \int h_Q(r)\Psi(r)\,d\vec{r}$

with $\Psi(r)$ a gravitational field.

This is the diffusive viewpoint, from which $K_{\alpha\beta}$ can be found.

More about this later maybe.