6. Linear response theory

6.1) Quantum many-body systems

Reference: Forster, "Hydrodynamic fluctuations, broken symmetry and correlation functions" (1975)

Up until this point, this course has only discussed the semiclassical theory of transport. The reason for this is that in large part, things that we know about transport come from this kinetic theory based formalism. For the rest of the course, we will discuss the quantum theory of transport, which may not be as useful for an everyday material but is universal.

We begin by quickly introducing the set up of the problem.

Many body quantum mechanics: Hilbert space

$$\mathcal{H} = \bigotimes_r \mathcal{H}_{el, r} \otimes \bigotimes_R \mathcal{H}_{ph, R} \otimes \bigotimes_R \mathcal{H}_{spins, R} \cdots$$

$\underbrace{\qquad}_{\text{electrons}}$ $\underbrace{\qquad}_{\text{phonons}}$ $\underbrace{\qquad}_{\text{spins, other local DOF?}}$

$\dim(\mathcal{H}) = e^N$ w/ N particles. (Bosons contribute an "uninteresting" $\infty \cdots$ problem is there are just so many states in the Hilbert space!)

Hamiltonian:

$$H = \sum \varepsilon_k c^\dagger_{k\alpha} c_{k\alpha} + \sum \omega_{q\alpha} a^\dagger_{q\alpha} a_{q\alpha}$$

$\underbrace{\qquad}_{\text{electron kinetic energy}}$ $\underbrace{\qquad}_{\text{phonon kinetic energy}}$

indices suppressed... $\longrightarrow$

$$+ \sum U c^\dagger c^\dagger c c + \sum \Delta a c^\dagger c + \sum \lambda a^\dagger a a$$

$\underbrace{\qquad}_{e-e \text{ interactions}}$ $\underbrace{\qquad}_{e-ph}$ $\underbrace{\qquad}_{ph-ph}$

$$+ \cdots$$

In kinetic theory, we treated the first line of the Hamiltonian — the non-interacting piece — as dominant. However, that may not be the case in a real system (especially in low density conductors, or so called "strange metals" which arise near a quantum critical point). So as much as possible, we will try to develop a formalism which does not rely on the series expansion above in phonon/electron operators. Put another way, we want to relax the assumption that "quasiparticles" exist — and describe transport phenomena and hydrodynamics in terms of local operators which are universal but may not obey a kinetic equation, even approximately.

In the absence of quasiparticles, what can we do?   Well, if we have a conserved charge, we could write down operators

$$\rho(\vec{x}), \quad \vec{J}(\vec{x}) \quad \text{are} \quad \underline{\text{LOCAL}} \quad \text{many-body operators!}$$

charge density ↗

charge current ↖

We still have transport! Ohm's Law will become an equation for the expectation value of this operator:

$$\langle J_i \rangle_E = \sigma_{ij} E_j + \cdots$$

where $\langle \cdots \rangle_E$ represents quantum expectation value in a quantum state perturbed by a small electric field. Usually in a many-body system the quantum state is described by a $\underline{\text{density matrix}}$ ρ_E

Density matrices obey the Schrödinger equation:

$$\frac{d}{dt} \rho = -i [H, \rho] . \qquad tr(\rho) = 1$$

and $\langle J_i \rangle_E = tr(\rho_E J_i)$, where ρ_E solves the Schrödinger equation with a weak external electric field added.

We will actually often find it easier to work not with quantum states, but with time evolved operators.   In this perspective, the quantum state stays fixed and the operator obeys the Heisenberg equation

$$\frac{d}{dt} O(t) = i [H, O(t)] \qquad \text{(relative sign change important!)}$$

$$\langle J_i \rangle_E = tr(\rho_0 J_i(t)) \qquad \text{is equivalent!}$$

We will almost always take the equilibrium density matrix to be thermal

$$\rho_0 = \frac{e^{-\beta H}}{Z(\beta)}, \quad Z(\beta) = tr(e^{-\beta H}) \quad , \quad \text{or possibly} \quad \rho_0 = \frac{e^{-\beta(H - \mu N)}}{Z(\beta, \mu)}$$

6.2) Time-dependent perturbation theory

The theory of transport is about weakly perturbing systems out of equilibrium by applying small perturbations to the original Hamiltonian. So let us discuss what happens to a quantum system in the presence of a very weak perturbation.

Consider a time-dependent Hamiltonian

$$H = H_0 + \lambda V(t), \qquad \lambda \text{ perturbatively small.}$$

We take $V(t) \to 0$ at $t < 0$, so that in the past, the system was undriven. We further assume the system was in equilibrium in the past, so that $\rho(t=0) = \rho_0 = \dfrac{e^{-\beta H_0}}{Z(\beta)}$.

Equivalently, as discussed, we can think about the density matrix remaining exactly thermal, while instead the operator picks up time dependence. Let us ask for the time evolution of

$$\langle O(t) \rangle = tr(\rho_0 \, O(t)) \, ?$$

Using time-dependent perturbation theory; time-ordered exponential

$$T \exp\left[-i\int_0^t dt' \, H(t)\right] = e^{-iH_0 t} - i\lambda \int_0^t dt' \, e^{-iH_0(t-t')} V(t') e^{-iH_0 t'} + O(\lambda^2)$$

$$\bar{T} \exp\left[i\int_0^t dt' \, H(t)\right] = e^{iH_0 t} + i\lambda \int_0^t dt' \, e^{iH_0 t'} V(t') e^{iH_0(t-t')}$$

$$tr\left(\rho_0 \, e^{iHt} O e^{-iHt}\right) = tr\left(\rho_0 \, e^{iH_0 t} O e^{-iH_0 t}\right)$$

$$+ i\lambda \, tr\left[\int_0^t dt' \left(\rho_0 \, e^{iH_0 t'} V(t') e^{iH_0(t-t')} O e^{-iH_0 t} - \rho_0 \, e^{iH_0 t} O e^{-iH_0(t-t')} V(t') e^{-iH_0 t'}\right)\right]$$

$$+ O(\lambda^2)$$

Now since $\rho_0 \sim e^{-\beta H_0}$ $\left[\rho_0, e^{\pm i H_0 t}\right]$, and so

$$\langle O(t)\rangle = \langle O\rangle + i\lambda \int_0^t dt' \langle e^{iH_0 t'}V(t')e^{iH_0(t-t')}O e^{-iH_0 t} - e^{iH_0 t}O e^{-iH_0(t-t')}V(t')e^{-iH_0 t'}\rangle$$

Using cyclic trace properties, and the fact that

$$O(t) = e^{iH_0 t}O e^{-iH_0 t} + O(\lambda)\ldots$$

$$\langle O(t)\rangle = \langle O\rangle + i\lambda \int_0^t dt' \langle [V(t'), O(t-t')]\rangle + O(\lambda^2)$$

where $[A,B] = AB - BA$

Let us now consider the following simple scenario.   Let's take the following perturbation

$$\lambda V(t') = -h(t')Q \leftarrow \text{fixed, time-independent operator.}$$

Then we may write

$$\langle O(t)\rangle - \langle O\rangle = \int_{-\infty}^{\infty} dt' \, G^R_{OQ}(t-t') h(t') \quad \text{where}$$

$$G^R_{OQ}(t) = i\langle [O(t), Q]\rangle \Theta(t) \quad \text{is the } \underline{\text{retarded Green's function.}}$$

The step function $\Theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}$ is conventionally

added to the Green's function here, so that we demand causality.

Note that in the presence of time translation invariance of the unperturbed Hamiltonian (necessary to have a thermal equilibrium!) the Green's function only depends on the difference of two times. This is a really useful fact for us, and we will use it to great effect as we go.

A final important point for us is that many quantum systems are defined with some kind of translation invariance in space, either discrete or continuous. So it is often useful to define the following

$$G^R_{OQ}(\vec{x}, t) = i \Theta(t) \langle [O(\vec{x}, t), Q(\vec{0}, 0)] \rangle$$

whenever we have a notion of a local operator in space (which, in this class, we always do: charge density/current etc.)

6.3) More Green's functions

Next, it will sometimes be useful for us to define other kinds of Green's functions, which we now list for completeness (some of them will start coming up frequently...)

advanced Green's function: $G^A_{OQ}(\vec{x}, t) = i \Theta(-t) \langle [O(\vec{x}, t), Q(\vec{0}, 0)] \rangle$

Spectral function: $\rho_{OQ}(\vec{x}, t) = \langle [O(\vec{x}, t), Q(\vec{0}, 0)] \rangle$

Symmetrized function: $S_{OQ}(\vec{x}, t) = \frac{1}{2} \langle \{O(\vec{x}, t), Q(\vec{0}, 0)\} \rangle$

where $\{A, B\} = AB + BA$

These are not independent. For example,

$$\rho_{OQ}(\vec{x}, t) = -i \left(G^R_{OQ} + G^A_{OQ} \right)$$

More important are the Kramers-Kronig relations that relate the spectral function to the Green's functions

Since $\quad i \Theta(t) = \int_{-\infty}^{\infty} \frac{dz}{2\pi} \frac{1}{z + i\varepsilon} e^{-izt}$ where $\varepsilon \to 0$ is a regulator ....

$$G^R_{OQ}(\vec{k}, \omega) = -\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{\rho_{OQ}(\vec{k}, \omega')}{\omega - \omega' + i\varepsilon}$$

Assuming time-reversal, $\rho_{OO}(\omega) = \rho_{OO}(-\omega)$. $\quad \text{Im} G^R_{OO}(\vec{k}, \omega) = \frac{1}{2} \rho_{OO}(\vec{k}, \omega)$

Next, let us discuss the susceptibility. We define the susceptibility "classically" as follows. If

$$H \rightarrow H - \int d^d x \, h \, O(\vec{k}),$$

$$\chi_{OO}^{(\vec{k})} = \frac{\partial \langle O(k) \rangle_h}{\partial h}\bigg|_{h=0}$$

Does this relate to Green's functions? It seems pretty similar, but let's make this idea precise.

For simplicity, we don't write out explicit k dependence below.

Let's regulate the matter by sending $h \rightarrow h e^{\varepsilon t}$ $(\varepsilon > 0)$ so that the perturbation dies off in the distant past. Now we apply linear response:

$$\langle O(t) \rangle = \int_{-\infty}^{t} dt' \, h \, e^{\varepsilon t'} G_{OO}^{R}(t-t') = \int_{-\infty}^{\infty} dt' \, h \, e^{\varepsilon t'} G_{OO}^{R}(t-t') \, \hookleftarrow$$

assume $\langle O \rangle = 0$ without loss of generality

$$\approx G_{OO}^{R}(\omega = -i\varepsilon) \, h$$

Therefore, $$\chi_{OO} \approx G_{OO}^{R}(\omega = 0) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\rho_{OO}(\omega)}{\omega}$$

Hence, the Green's functions at low frequency encode classical thermodynamic coefficients!

In some cases, it can be useful to relate susceptibilities and spectral functions of similar operators. For example,

$$\text{If } R = i[H, O] = \frac{\partial O}{\partial t}, \quad \chi_{RR} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega \, \rho_{OO}(\omega), \quad \text{or}$$

$$G_{RO}^{R}(t) = \frac{d}{dt} G_{OO}^{R}(t) \quad (\text{for } t>0) \Rightarrow -i\omega G_{OO}^{R} = G_{RO}^{R}$$

$$\rho_{OO}(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} (-i\omega)^n \rho_{OO}(\omega)$$

6.4) Spectral representations

Let's now focus a little bit more on the spectral function. Suppose we managed to exactly diagonalize the many body Hamiltonian...

$$H|\alpha\rangle = E_\alpha |\alpha\rangle.$$

Then
$$\rho_{OO}(\omega) = \int_{-\infty}^{\infty} dt \, e^{i\omega t} \langle [O(t), O] \rangle$$

$$= \frac{1}{Z(\beta)} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \, tr\left(e^{-\beta H} [e^{iHt} O e^{-iHt}, O] \right)$$

Insert two resolutions of the identity $\mathbb{1} = \sum_\alpha |\alpha\rangle\langle\alpha|$:

$$\rho_{OO}(\omega) = \frac{1}{Z(\beta)} \sum_{\alpha,\beta} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \, tr\left(e^{-\beta E_\alpha + i E_\alpha t} |\alpha\rangle\langle\alpha|O|\beta\rangle\langle\beta|e^{-iE_\beta t} O \right.$$

$$\left. - e^{-\beta E_\alpha} |\alpha\rangle\langle\alpha|O|\beta\rangle\langle\beta|e^{iE_\beta t} O e^{-iE_\alpha t} \right)$$

$$= \frac{1}{Z(\beta)} \sum_{\alpha,\beta} |\langle\alpha|O|\beta\rangle|^2 \int_{-\infty}^{\infty} dt \, e^{i(\omega + E_\alpha - E_\beta)t} \left(e^{-\beta E_\alpha} - e^{-\beta E_\beta} \right)$$

$$= \frac{2\pi}{Z(\beta)} \sum_{\alpha,\beta} |\langle\alpha|O|\beta\rangle|^2 \delta(E_\alpha - E_\beta + \omega) e^{-\beta E_\alpha} (1 - e^{-\beta\omega})$$

Now observe: $\omega\rho_{OO}(\omega) = \frac{4\pi}{Z(\beta)} \sum_{\alpha,\beta} |\langle\alpha|O|\beta\rangle|^2 \delta(E_\alpha - E_\beta + \omega) e^{-\beta(E_\alpha + \frac{\omega}{2})} \omega \sinh\frac{\beta\omega}{2}$

$$\geq 0$$

The spectral function is, in this sense, positive. This positivity constraint ensures the stability of thermal equilibrium, as we will see shortly.

6.5) Fluctuation-dissipation theorem

Now we come to a very important result that relates two of the Green's functions we have found thus far.

For simplicity, define operators such that $\langle O \rangle = \langle Q \rangle = 0$
(can just take $O \to O - \langle O \rangle$)

Now consider $S_{OQ}(t) = \frac{1}{2}\langle O(t)Q + QO(t)\rangle$

$$= \frac{1}{2Z}\text{tr}\left(e^{-\beta H}e^{itH}Oe^{-iHt}Q + e^{-\beta H}Qe^{itH}Oe^{-iHt}\right)$$

$$= \frac{1}{2Z}\text{tr}\left(e^{-\beta H}\left(O(t)Q + e^{(it+\beta)H}Oe^{-(it+\beta)H}Q\right)\right)$$

$$= \frac{1}{2}\langle O(t)Q + O(t-i\beta)Q\rangle$$

Similarly, $\rho_{OQ} = \langle[O(t),Q]\rangle = \langle O(t)Q - O(t-i\beta)Q\rangle$.

Hence $2S_{OQ} + \rho_{OQ} = 2\langle O(t)Q\rangle$; $2S_{OQ} - \rho_{OQ} = 2\langle O(t-i\beta)Q\rangle$

Now take the Fourier transform:

$$\langle O(t)Q\rangle \to \langle O(\omega)Q\rangle ; \langle O(t-i\beta)Q\rangle \to \langle O(\omega)Q\rangle \times e^{i\omega(i\beta)}$$

$$\Rightarrow 2\rho_{OQ}(\omega) = 2(1-e^{-\beta\omega})\langle O(\omega)Q\rangle.$$

$$\Rightarrow S_{OQ}(\omega) = \frac{1}{2}\frac{1+e^{-\beta\omega}}{1-e^{-\beta\omega}}\rho_{OQ}(\omega) = \frac{1}{2}\coth\frac{\beta\omega}{2}\rho_{OQ}(\omega)$$

This is the quantum mechanical version of the fluctuation dissipation theorem!

Fluctuations: $\langle O(t) O \rangle + \langle O O(t) \rangle \sim \langle O(t) O \rangle$ (w/ time reversal)

Dissipation: $\langle [O(t), Q] \rangle$, since... (show as HW)

work done on system $= \int \frac{d\omega}{2\pi} \omega \rho_{OO}(\omega) |h(\omega)|^2$

by $H \to H - h(t) O$

6.6) Formal definition of transport coefficients

At this time, we are now ready to provide a formal definition of transport coefficients. Let's begin by thinking about the electric field.

$$\vec{E} = -\nabla \phi - \frac{\partial \vec{A}}{\partial t}$$

electric potential ↑ — vector potential

We can source an electric field in two ways in a quantum system, either by the gradient of the potential (usually what we implicitly have in mind) or better, by a vector potential. Why is this approach better? Well consider that the

$$H \to H - \int d^d x \left(\rho \phi + \vec{J} \cdot \vec{A} \right)$$

(under perturbations by a <u>fixed</u>, <u>non-dynamical</u> electromagnetic field

It seems more natural to try and directly drive the current rather than drive the density — although we could do both and would arrive at the same answer in the end.

To apply a fixed electric field, we will consider

$$\boxed{\vec{A} = -\vec{E} t}$$

Assuming $\langle \vec{J} \rangle = 0$ in equilibrium...

$$\langle J_i(t) \rangle = \int_{-\infty}^{t} dt' \, G^R_{J_i J_j}(t-t') \times (-E_j t')$$

In fourier space:

$$\langle J_i(\omega) \rangle = G^R_{J_i J_j}(\omega) E_j \times \underbrace{\int_{-\infty}^{\infty} dt' \, e^{i\omega t'} (-t')}_{= 2\pi i \delta'(\omega)}$$

Going back to real time....

$$\langle J_i(t) \rangle = E_j \times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \left[2\pi i \, \delta'(\omega) \, G^R_{J_i J_j}(\omega) e^{-i\omega t} \right]$$

$$= -iE_j \frac{\partial}{\partial \omega} \left[G^R_{J_i J_j}(\omega) e^{-i\omega t} \right]\Big|_{\omega=0}$$

$$= -t E_j \, G^R_{J_i J_j}(0) - E_j \, i \frac{\partial G^R}{\partial \omega}\Big|_{\omega \to 0}$$

$\underbrace{\phantom{-t E_j \, G^R_{J_i J_j}(0)}}$ this term represents the <u>susceptibility</u> of the current, and is a thermodynamic response....

$\underbrace{\phantom{-E_j \, i \frac{\partial G^R}{\partial \omega}}}$ interesting time-independent response.... .

We conclude that the direct current conductivity is

$$\sigma_{dc} = -i \frac{\partial G^R}{\partial \omega}\Big|_{\omega \to 0}$$

This makes some sense, because conductivity is <u>dissipative</u> so it should relate to the imaginary part of G^R. We define a frequency dependent conductivity

$$\sigma_{ij}(\omega) = \frac{G^R_{J_i J_j}(\omega) - G^R_{J_i J_j}(0)}{i\omega}$$

$$\begin{pmatrix} J \\ Q \end{pmatrix} = \begin{pmatrix} \sigma & T\alpha \\ T\tilde{\alpha} & T\bar{\kappa} \end{pmatrix} \begin{pmatrix} E \\ -\nabla T \end{pmatrix}$$

We can similarly define:

$$T\alpha_{ij}(\omega) = \frac{G^R_{J_i Q_j}(\omega) - G^R_{J_i Q_j}(0)}{i\omega}$$

$$T\bar{\kappa}_{ij}(\omega) = \frac{G^R_{Q_i Q_j}(\omega) - G^R_{Q_i Q_j}(0)}{i\omega}$$

6.7) Quantum transport of free fermions

Consider the many-body Hamiltonian of free fermions.

$$H = \sum \varepsilon_a c_a^\dagger c_a$$

a = wave number, band, spin....

$$\{c_a^\dagger, c_b\} = \delta_{ab}$$

Let's evaluate $P_{J_x J_x}(\omega)$, rather than G^R, as we already calculated

$$P_{J_x J_x}(\omega) = \frac{2\pi}{Z(\beta)} \sum_{\alpha,\beta} |\langle \alpha | J_x | \beta \rangle|^2 \delta(E_\alpha - E_\beta + \omega)\left(e^{-\beta E_\alpha} - e^{-\beta E_\beta}\right)$$

$\underset{\text{many body eigenstates.}}{\curvearrowleft}$

For free fermions,

$$|\alpha\rangle = \bigotimes_a |n_a\rangle \quad , \quad \text{where} \quad n_a = 0 \text{ or } 1, \quad \text{and}$$

$$E_\alpha = \sum_a \varepsilon_a n_\alpha.$$

Hence,

$$Z(\beta) = \sum_\alpha e^{-\beta E_\alpha} = \prod_a \left(1 + e^{-\beta \varepsilon_a}\right)$$

Now assume that the charge current operator $J_x = \sum_{a \neq b} J_{ab} c_a^\dagger c_b$

mobile fermions

J_{ab}

a b
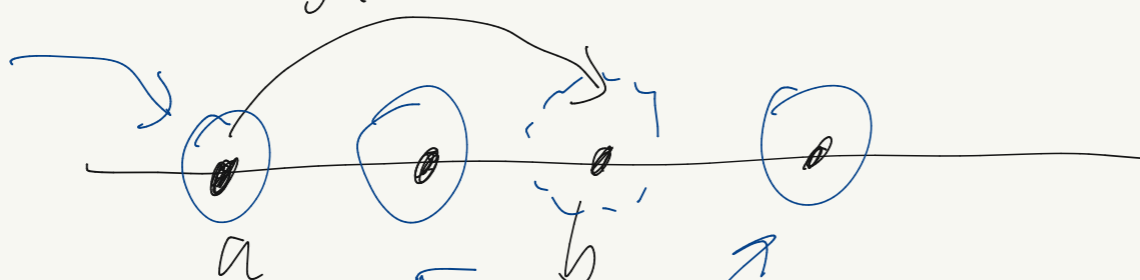
untouched fermions!

So $J_x |\beta\rangle = J_x |n_1, n_2 \ldots\rangle = \sum_{ab} J_{ab} \delta_{n_a, 0} \delta_{n_b, 1} |n_1, n_2 \ldots 1 \ldots 0 \ldots\rangle$

$$\langle \alpha | J_x | \beta \rangle = \sum_{ab} J_{ab} \times \left\{ \prod_{c \neq a,b} \delta_{n_c^\alpha, n_c^\beta} \right\} \delta_{n_a^\alpha, 1} \delta_{n_a^\beta, 0} \delta_{n_b^\alpha, 0} \delta_{n_b^\beta, 1}$$

$$P_{xx}(\omega) = 2\pi \sum_{a,b} |J_{ab}|^2 \sum_{\substack{n_c = 0,1, \\ c \neq a,b}} \frac{\left(e^{-\beta E_\alpha} - e^{-\beta E_\beta} \right) \delta(E_\alpha - E_\beta + \omega)}{Z(\beta)}$$

$$= 2\pi \sum_{a,b} |J_{ab}|^2 \frac{\delta(\varepsilon_a - \varepsilon_b + \omega)}{(1 + e^{-\beta\varepsilon_a})(1 + e^{-\beta\varepsilon_b})} \left(e^{-\beta\varepsilon_a} - e^{-\beta\varepsilon_b} \right)$$

$$= 2\pi \sum_{a,b} |J_{ab}|^2 \, \delta(\varepsilon_a - \varepsilon_b + \omega) \left(f_F(\varepsilon_a) - f_F(\varepsilon_b) \right)$$

DC conductivity $\quad \sigma_{xx}(0) = \left. \frac{1}{2\omega} P_{xx}(\omega) \right|_{\omega \to 0}$

$$= \pi \sum_{a,b} |J_{ab}|^2 \, \delta(\varepsilon_a - \varepsilon_b + \omega) \frac{f_F(\varepsilon_a) - f_F(\varepsilon_a + \omega)}{\omega}$$

$$\to \pi \sum_{a,b} \delta(\varepsilon_a - \varepsilon_b) \left(-\frac{\partial f_F}{\partial \varepsilon_a} \right) |J_{ab}|^2$$

This formula is extremely similar to what we saw in kinetic theory in our treatment of electron-impurity scattering! In a sense, what kinetic theory approximated for us was the value of the current operator in the exact energy eigenstates, in terms of approximate eigenstates (in the absence of the impurities)