Linear Response Theory: The connection between QFT and experiments

4.1. Basic concepts and ideas

Q: How do we measure the conductivity of a metal?

A: If we introduce a weak electric field $E$, and then measure the electric current $J$. In general, $J$ is a function of $E$, and then we can make a Taylor expansion for this function

$$J(E) = J(E = 0) + J'(E = 0) E + \frac{1}{2!} J''(E = 0) E^2 + \ldots$$

(4.1)

Symmetry tells us that when $E = 0$, $J = 0$, so the first term in the equation above is zero. And therefore, the leading order term is the linear term of $E$. If we ignore all higher order terms beyond the leading order one, we get a linear relation between $J$ and $E$

$$J = \sigma E$$

(4.2)

At the end of the day, we find that as long as $E$ is weak enough, $J$ shall be proportional to $E$ and the coefficient is the conductivity. Because $J$ is a linear function of $E$ at small $E$, the weak $E$ limit is also known as the linear response regime.

The philosophy described above applies to many experimental techniques. Very typically, in an experiment we first introduce a small perturbation (at time $t$) to the system and then we wait and see how the system response to this perturbation at a later time ($t' > t$). If the perturbation is weak enough, the response of the system is a linear function of the perturbation, and we say that the experiment is done in the linear response regime. In the linear response regime, we can compute the slope of the linear function (i.e. the measurement of the experiment) using quantum field theory. This type of calculation is known as the linear response theory.

4.2. Linear Response Theory

4.2.1. the density matrix and its time-evolution

If we want to measure the expectation of the quantum operator (say $\hat{B}$), the quantum statistical mechanics tells us that at temperature $T = 1/\beta$, this is what we will get (see Sec. 1.1 for details)

$$\langle B \rangle = \frac{\sum_n \langle n | \hat{B} \exp[-\beta(\hat{H} - \mu \hat{N})] | n \rangle}{\sum_n \langle n | \exp[-\beta(\hat{H} - \mu \hat{N})] | n \rangle} = \frac{\text{Tr} \{ \hat{B} \exp[-\beta(\hat{H} - \mu \hat{N})] \}}{\text{Tr} \{ \exp[-\beta(\hat{H} - \mu \hat{N})] \}}$$

(4.3)

Another way to write the same formula is to define the so-called density matrix

$$\hat{\rho} = \frac{1}{\text{Tr} \{ \exp[-\beta(\hat{H} - \mu \hat{N})] \}} \exp[-\beta(\hat{H} - \mu \hat{N})] = \exp[-\beta(\hat{H} - \mu \hat{N} - \Omega)]$$

(4.4)

The prefactor $\frac{1}{\text{Tr} \{ \exp[-\beta(\hat{H} - \mu \hat{N})] \}}$ is a number, which is just a renormalization factor. We can absorb it into the exponential

$$\hat{\rho} = \exp[-\beta(\hat{H} - \mu \hat{N} - \Omega)]$$

(4.5)
where

$$\Omega = - \frac{1}{\beta} \ln \text{Tr} \left\{ \exp \left[ - \beta (\hat{H} - \mu \hat{N}) \right] \right\}$$  \quad (4.6)$$

and $\Omega$ is known as the grand potential in statistical physics.

Using $\hat{\rho}$, we find that

$$\langle B \rangle = \text{Tr} \left\{ \hat{B} \hat{\rho} \right\}$$  \quad (4.7)$$

Now, we consider a system described by the Hamiltonian $H$ and we perturb this system, so that the new Hamiltonian is

$$\hat{H}_{\text{total}} = \hat{H} + V(t) \hat{A}$$  \quad (4.8)$$

The perturbation includes two factors, a Hermitian quantum operator $\hat{A}$ and its coefficient (a real number) $V(t)$. $V(t)$ satisfies the condition that at $t = -\infty$, it is zero,

$$V(t \to -\infty) \to 0$$  \quad (4.9)$$

In other words, first we have a system described by the Hamiltonian $H$, then we turn on a perturbation $V(t) \hat{A}$.

Here we use the Heisenberg picture, so that the quantum states do not change with time and all the time-evolutions come from quantum operators.

$$\langle \hat{B}(t) \rangle = \sum_n \langle n | \hat{B}(t) \hat{\rho}(t) | n \rangle$$  \quad (4.10)$$

The time-evolution of the quantum operator $\hat{B}(t)$ is straightforward. It just follow the time-evolution of $\hat{H}_{\text{total}}$. We can define the time-evolution operator

$$\hat{U}_{\text{total}}(t, -\infty) = T \exp \left[ - \frac{i}{\hbar} \int_{-\infty}^{t} \left( \hat{H} + V(t') \hat{A} \right) d t' \right]$$  \quad (4.11)$$

And then, we know that

$$\hat{B}(t) = \hat{U}_{\text{total}}(t, -\infty) \hat{B}_S \hat{U}_{\text{total}}(t, -\infty)$$  \quad (4.12)$$

where $\hat{B}_S$ is the same operator in the Schrödinger picture.

As shown above, the density matrix $\hat{\rho}$ is determined by the Hamiltonian. Here, we have two Hamiltonians, the full Hamiltonian $\hat{H}_{\text{total}} = \hat{H} + V(t) \hat{A}$ and the unperturbed Hamiltonian $\hat{H}$. **Which one shall we use for $\hat{\rho}$?** The answer is a bit counter intuitive. Instead of the full Hamiltonian, here, we should use the unperturbed part $\hat{H}$. This is because the density matrix comes from statistical mechanism. At time $t = -\infty$, before we turn on the perturbation, the system reaches thermal equilibrium for the unperturbed Hamiltonian $\hat{H}$. Then, after we turn on the perturbation $V(t) \hat{A}$, the system doesn’t have enough time to reach a new thermal equilibrium (for the new Hamiltonian $\hat{H}_{\text{total}} = \hat{H} + V(t) \hat{A}$). Instead, when we consider the statistical weight for each quantum state, we should use the weight for the original Hamiltonian $\hat{H}$, instead of the unperturbed one $\hat{H}_{\text{total}}$. There are two direct consequence for this. (1) $\langle \hat{\rho}, \hat{H} \rangle = 0$ and (2) the time-evolution of $\hat{\rho}$ is determined by the unperturbed Hamiltonian $\hat{H}$, instead of $\hat{H}_{\text{total}}$, i.e.,

$$\dot{\hat{\rho}}(t) = \hat{U}_{\hat{H}}(t, -\infty) \hat{\rho}_{\hat{S}} \hat{U}_{\hat{H}}(t, -\infty)$$  \quad (4.13)$$

where

$$\hat{U}_{\hat{H}}(t, -\infty) = T \exp \left[ - \frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} d t' \right]$$  \quad (4.14)$$

**In summary**, here we emphasize again that quantum mechanics and quantum statistical physics have two totally different time scales. For quantum mechanics, the dynamics of a quantum operator changes instantaneous. If we perturb a Hamiltonian, a quantum operator knows it immediately and its time-evolution is determined by the full Hamiltonian $\hat{H}_{\text{total}} = \hat{H} + V(t) \hat{A}$, immediately after we turn on the perturbation. On the other hand, the time scale in quantum statistical physics is much slower. When we perturb a quantum system, it will take the system a long time to reach new equilibrium. Therefore, shortly after we perturb the system, we still use the unperturbed Hamiltonian to compute thermal average.
4.2.2. time-evolution of $\hat{B}(t)$

Now, we know that

$$\{\hat{B}(t)\} = \text{Tr}\left(\hat{\mathcal{U}}_{\text{total}}(t, -\infty) \hat{B}_S \hat{\mathcal{U}}_{\text{total}}(t, -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t, -\infty)\right)$$

(4.15)

If the perturbation $V(t) \hat{A}$ is weak enough, we can use the approximation $e^x = 1 + x + O(x^2)$ and thus

$$\hat{\mathcal{U}}_{\text{total}}(t, -\infty) = \text{Tr}\left[\exp\left(-\frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} dt'\right)\right] = \text{Tr}\left[\exp\left(-\frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} dt'\right)\right] + O(V^2)$$

(4.16)

Because the time-evolution operator requires the time ordering (operators with smaller $t$ should be placed on the right side), we find that

$$\hat{\mathcal{U}}_{\text{total}}(t, -\infty) = \text{Tr}\left[\exp\left(-\frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} dt'\right)\right] - \frac{i}{\hbar} \int_{-\infty}^{t} dt'' \left[\text{exp}\left(-\frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} dt'\right) V(t'') \hat{A} \text{exp}\left(-\frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} dt'\right) \right] + O(V^2)$$

(4.17)

In the last step, we used the fact that $\text{Tr}\left[\exp\left(-\frac{i}{\hbar} \int_{-\infty}^{t} \hat{H} dt\right)\right]$ is just the time evolution operator for the unperturbed Hamiltonian $\hat{H}$.

Similarly,

$$\hat{\mathcal{U}}_{\text{total}}(t, -\infty)^\dagger = \hat{\mathcal{U}}_{\text{total}}(t, -\infty)^\dagger + \frac{i}{\hbar} \int_{-\infty}^{t} dt'' \left[\hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger V(t'') \hat{A} \hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger \right] + O(V^2)$$

(4.18)

As a result,

$$\{\hat{B}(t)\} = \text{Tr}\left(\hat{\mathcal{U}}_{\text{total}}(t, -\infty)^\dagger \hat{B}_S \hat{\mathcal{U}}_{\text{total}}(t, -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t, -\infty)\right) +$$

$$- \frac{i}{\hbar} \int_{-\infty}^{t} dt'' V(t'') \text{Tr}\left[\hat{B}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)\right]$$

$$- \frac{i}{\hbar} \int_{-\infty}^{t} dt'' V(t'') \text{Tr}\left[\hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)\right]$$

(4.19)

Here, we used the facts that $\{\hat{U}_S\} = \{\hat{U}_S\}$ and $[\hat{\rho}, \hat{H}] = 0$. Because $[\hat{\rho}, \hat{H}] = 0$, $[\hat{\rho}, \hat{\rho}_S] = [\hat{\rho}, (\hat{U}_S)^\dagger] = 0$ and thus we can switch the order for $\hat{\rho}$ and the time-evolution operators. The first term in the formula above is the expectation value of $\hat{B}(t)$ for the unperturbed Hamiltonian.

$$\{\hat{B}(t)\} = \{\hat{B}(t)\}_H + \frac{i}{\hbar} \int_{-\infty}^{t} dt'' V(t'') \text{Tr}\left[\hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)\right]$$

$$- \frac{i}{\hbar} \int_{-\infty}^{t} dt'' V(t'') \text{Tr}\left[\hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)\right]$$

$$= \{\hat{B}(t)\}_H + \frac{i}{\hbar} \int_{-\infty}^{t} dt'' V(t'') \text{Tr}\left[\hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)^\dagger \hat{\rho}_S \hat{\mathcal{U}}_{\text{total}}(t', -\infty)\right]$$

$$+ O(V^2)$$

(4.20)
Here, all the expectation values are computed for the unperturbed Hamiltonian $\hat{H}$, $(\ldots)_{\hat{H}}$. Very typically, $\langle \hat{B}(t) \rangle_{\hat{H}} = 0$, i.e. the quantity that we measure in an experimental is zero before we turn on the perturbation, and therefore

$$\langle \hat{B}(t) \rangle = \frac{i}{\hbar} \int_{-\infty}^{\infty} dt' V(t') \langle \hat{A}(t'), \hat{B}(t) \rangle_{\hat{H}} + O(V^2)$$

(4.21)

To the leading order, the measurable quantity $\langle \hat{B}(t) \rangle$ is proportional to the perturbation $V(t')$, and thus this is known as the linear response theory. To compute the non-linear response, one needs to go to higher order in the above expansion, which will not be considered in this lecture.

In the linear response regime, the measurement is proportional to the perturbation. The coefficient of this linear relation is $\langle \hat{A}(t'), \hat{B}(t) \rangle_{\hat{H}}$, which only depends on the unperturbed Hamiltonian. In other words, the linear-response measurement measures the intrinsic properties of the system.

### 4.3. Linear Response Theory and the Susceptibility

#### 4.3.1. Generalized Susceptibility

In general, the perturbation and observation discussed in the previous section can also have spatial dependence, i.e., the $\hat{A}$ and $\hat{B}$ operator can depend on the real space coordinate. There, the more general linear response theory takes the following form (the deviation is the same and we ignore higher order non-linear terms).

$$\langle \hat{B}(x, t) \rangle = \frac{i}{\hbar} \int d\tilde{x}' \int_{-\infty}^{t} dt' V(\tilde{x}', t') \langle \hat{A}(\tilde{x}', t'), \hat{B}(x, t) \rangle_{\hat{H}} = \int d\tilde{x}' \int_{-\infty}^{t} dt' \frac{i}{\hbar} (t - t') \langle \hat{A}(\tilde{x}', t'), \hat{B}(x, t) \rangle_{\hat{H}} V(\tilde{x}', t')$$

(4.22)

Here, in the last step, we change the upper bound for the time integral from $t$ to $+\infty$. In the same time, we added an step function $\theta(t - t')$

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

(4.23)

so the formula remains the same. From now on, we will drop the sub-index $\hat{H}$ for expectation values $(\ldots)_{\hat{H}}$. In other words, all the expectation values computed in this section are for the original Hamiltonian $\hat{H}$, without the small perturbation.

We can define the generalized susceptibility

$$\chi(x, t; \tilde{x}', t') = \frac{i}{\hbar} \theta(t - t') \langle \hat{A}(\tilde{x}', t'), \hat{B}(x, t) \rangle$$

(4.24)

Please pay special attention to this step function $\theta(t - t')$. We need it here, because the time integral requires $t' < t$. As will be discussed below, this implies causality.

It is easy to show that

$$\langle \hat{B}(x, t) \rangle = \int d\tilde{x}' d t' \chi(x, t; \tilde{x}', t') V(\tilde{x}', t')$$

(4.25)

Please notice that the time integral now is from $-\infty$ to $+\infty$.

In other words, we can describe our perturbation (input) as a function $V(\tilde{x}', t')$. This function measures the strength of our perturbation at time $t'$ and at the location $\tilde{x}'$. Then we measure the output, which is also a function of space and time $\langle \hat{B}(x, t) \rangle$, i.e. our measurable quantity measure at the time $t$ and the position $x$. The generalised susceptibility tells us the connection between the input and the output. For any given input, the integral above tells us immediately what output we shall expect.

**NOTE:** In the definite of the generalised susceptibility, a step function of time arises. This step function is actually expected and must be there, because it implies causality (if the step function is not there, our theory must be wrong, because it violate causality). The step function tells us that the response will be nonzero, only if $t > t'$. Notice that the input (the perturbation) is applied at $t'$ and we are measuring the result at $t$. This step function actually implies that for measurement at time $t$, only inputs before this time point contribute to the measurement, which is known as causality.

#### 4.3.2. The Frequency Space

Now, we convert the linear response theory obtained above into the frequency space. There are two motivations for this:

- It simplifies the formula, as will be shown below