

4. Linear Response

The goal of response theory is to figure out how a system reacts to outside influences. These outside influences are things like applied electric and magnetic fields, or applied pressure, or an applied driving force due to some guy sticking a spoon into a quantum liquid and stirring.

We've already looked at a number of situations like this earlier in the course. If you apply a shearing force to a fluid, its response is to move; how much it moves is determined by the viscosity. If you apply a temperature gradient, the response is for heat to flow; the amount of heat is determined by the thermal conductivity. However, in both of these cases, the outside influence was time independent. Our purpose here is to explore the more general case of time dependent influences. As we'll see, by studying the response of the system at different frequencies, we learn important information about what's going on inside the system itself.

4.1 Response Functions

Until now, our discussion in this course has been almost entirely classical. Here we want to deal with both classical and quantum worlds. For both cases, we start by explaining mathematically what is meant by an outside influence on a system.

Forces in Classical Dynamics

Consider a simple dynamical system with some generalized coordinates $x_i(t)$ which depend on time. If left alone, these coordinates will obey some equations of motion,

$$\ddot{x}_i + g_i(\dot{x}, x) = 0$$

This dynamics need not necessarily be Hamiltonian. Indeed, often we'll be interested in situations with friction. The outside influence in this example arises from perturbing the system by the addition of some driving forces $F_i(t)$, so that the equations of motion become,

$$\ddot{x}_i + g_i(\dot{x}, x) = F_i(t) \tag{4.1}$$

In this expression, $x_i(t)$ are dynamical degrees of freedom. This is what we're solving for. In contrast, $F_i(t)$ are *not* dynamical: they're forces that are under our control, like someone pulling on the end of a spring. We get to decide on the time dependence of each $F_i(t)$.

It may be useful to have an even more concrete example at the back of our minds. For this, we take every physicist's favorite toy: the simple harmonic oscillator. Here we'll include a friction term, proportional to γ , so that we have the damped harmonic oscillator with equation of motion

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x = F(t) \quad (4.2)$$

We will discuss this model in some detail in section 4.2.

Sources in Quantum Mechanics

In quantum mechanics, we introduce the outside influences in a slightly different manner. The observables of the system are now operators, \mathcal{O}_i . We'll work in the Heisenberg picture, so that the operators are time dependent: $\mathcal{O} = \mathcal{O}(t)$. Left alone, the dynamics of these operators will be governed by a Hamiltonian $H(\mathcal{O})$. However, we have no interest in leaving the system alone. We want to give it a kick. Mathematically this is achieved by adding an extra term to the Hamiltonian,

$$H_{\text{source}}(t) = \phi_i(t)\mathcal{O}_i(t) \quad (4.3)$$

The $\phi_i(x)$ are referred to as *sources*. They are external fields that are under our control, analogous to the driving forces in the example above. Indeed, if we take a classical Hamiltonian and add a term of the form $x\phi$ then the resulting Euler-Lagrange equations include the source ϕ on the right-hand-side in the same way that the force F appears in (4.2).

4.1.1 Linear Response

We want to understand how our system reacts to the presence of the source or the driving force. To be concrete, we'll chose to work in the language of quantum mechanics, but everything that we discuss in this section will also carry over to classical systems. Our goal is to understand how the correlation functions of the theory change when we turn on a source (or sources) $\phi_i(x)$.

In general, it's a difficult question to understand how the theory is deformed by the sources. To figure this out, we really just need to sit down and solve the theory all over again. However, we can make progress under the assumption that the source is a small perturbation of the original system. This is fairly restrictive but it's the simplest place where we can make progress so, from now on, we focus on this limit. Mathematically, this means that we assume that the change in the expectation value of any operator is *linear* in the perturbing source. We write

$$\delta\langle\mathcal{O}_i(t)\rangle = \int dt' \chi_{ij}(t;t')\phi_j(t') \quad (4.4)$$

Here $\chi_{ij}(t; t')$ is known as a *response function*. We could write a similar expression for the classical dynamical system (4.1), where $\delta\langle\mathcal{O}_i\rangle$ is replaced by $x_i(t)$ and ϕ is replaced by the driving force $F_j(t)$. In classical mechanics, it is clear from the form of the equation of motion (4.1) that the response function is simply the Green's function for the system. For this reason, the response functions are often called Green's functions and you'll often see them denoted as G instead of χ .

From now on, we'll assume that our system is invariant under time translations. In this case, we have

$$\chi_{ij}(t; t') = \chi_{ij}(t - t')$$

and it is useful to perform a Fourier transform to work in frequency space. We define the Fourier transform of the function $f(t)$ to be

$$f(\omega) = \int dt e^{i\omega t} f(t) \quad \text{and} \quad f(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} f(\omega) \quad (4.5)$$

In particular, we will use the convention where the two functions are distinguished only by their argument.

Taking the Fourier transform of (4.4) gives

$$\begin{aligned} \delta\langle\mathcal{O}_i(\omega)\rangle &= \int dt' \int dt e^{i\omega t} \chi_{ij}(t - t') \phi_j(t') \\ &= \int dt' \int dt e^{i\omega(t-t')} \chi_{ij}(t - t') e^{i\omega t'} \phi_j(t') \\ &= \chi_{ij}(\omega) \phi_j(\omega) \end{aligned} \quad (4.6)$$

We learn the response is “local” in frequency space: if you shake something at frequency ω , it responds at frequency ω . Anything beyond this lies within the domain of non-linear response.

In this section we'll describe some of the properties of the response function $\chi(\omega)$ and how to interpret them. Many of these properties follow from very simple physical input. To avoid clutter, we'll mostly drop both the i, j indices. When there's something interesting to say, we'll put them back in.

4.1.2 Analyticity and Causality

If we work with a real source ϕ and a Hermitian operator \mathcal{O} (which means a real expectation value $\langle\mathcal{O}\rangle$) then $\chi(t)$ must also be real. Let's see what this means for the

Fourier transform $\chi(\omega)$. It's useful to introduce some new notation for the real and imaginary parts,

$$\begin{aligned}\chi(\omega) &= \text{Re } \chi(\omega) + i\text{Im } \chi(\omega) \\ &\equiv \chi'(\omega) + i\chi''(\omega)\end{aligned}$$

This notation in terms of primes is fairly odd the first time you see it, but it's standard in the literature. You just have to remember that, in this context, primes do not mean derivatives!

The real and imaginary parts of the response function $\chi(\omega)$ have different interpretations. Let's look at these in turn

- **Imaginary Part:** We can write the imaginary piece as

$$\begin{aligned}\chi''(\omega) &= -\frac{i}{2}[\chi(\omega) - \chi^*(\omega)] \\ &= -\frac{i}{2} \int_{-\infty}^{+\infty} dt \chi(t)[e^{i\omega t} - e^{-i\omega t}] \\ &= -\frac{i}{2} \int_{-\infty}^{+\infty} dt e^{i\omega t}[\chi(t) - \chi(-t)]\end{aligned}$$

We see that the imaginary part of $\chi(\omega)$ is due to the part of the response function that is *not* invariant under time reversal $t \rightarrow -t$. In other words, $\chi''(\omega)$ knows about the arrow of time. Since microscopic systems are typically invariant under time reversal, the imaginary part $\chi''(\omega)$ must be arising due to dissipative processes.

$\chi''(\omega)$ is called the *dissipative* or *absorptive* part of the response function. It is also known as the *spectral function*. It will turn out to contain information about the density of states in the system that take part in absorptive processes. We'll see this more clearly in an example shortly.

Finally, notice that $\chi''(\omega)$ is an odd function,

$$\chi''(-\omega) = -\chi''(\omega)$$

- **Real Part:** The same analysis as above shows that

$$\chi'(\omega) = \frac{1}{2} \int_{-\infty}^{+\infty} dt e^{i\omega t}[\chi(t) + \chi(-t)]$$

The real part doesn't care about the arrow of time. It is called the *reactive* part of the response function. It is an even function,

$$\chi'(-\omega) = +\chi'(\omega)$$

Before we move on, we need to briefly mention what happens when we put the labels i, j back on the response functions. In this case, a similar analysis to that above shows that the dissipative response function comes from the anti-Hermitian part,

$$\chi''_{ij}(\omega) = -\frac{i}{2}[\chi_{ij}(\omega) - \chi_{ji}^*(\omega)] \quad (4.7)$$

Causality

We can't affect the past. This statement of causality means that any response function must satisfy

$$\chi(t) = 0 \quad \text{for all } t < 0$$

For this reason, χ is often referred to as the causal Green's function or *retarded Green's function* and is sometimes denoted as $G_R(t)$. Let's see what this simple causality requirement means for the Fourier expansion of χ ,

$$\chi(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi(\omega)$$

When $t < 0$, we can perform the integral by completing the contour in the upper-half plane (so that the exponent becomes $-i\omega \times (-i|t|) \rightarrow -\infty$). The answer has to be zero.

Of course, the integral is given by the sum of the residues inside the contour. So if we want the response function to vanish for all $t < 0$, it must be that $\chi(\omega)$ has no poles in the upper-half plane. In other words, causality requires:

$$\chi(\omega) \text{ is analytic for } \text{Im } \omega > 0$$

4.1.3 Kramers-Kronig Relation

The fact that χ is analytic in the upper-half plane means that there is a relationship between the real and imaginary parts, χ' and χ'' . This is called the Kramers-Kronig relation. Our task in this section is to derive it. We start by providing a few general mathematical statements about complex integrals.

A Discontinuous Function

First, consider a general function $\rho(\omega)$. We'll ask that $\rho(\omega)$ is meromorphic, meaning that it is analytic apart from at isolated poles. But, for now, we won't place any restrictions on the position of these poles. (We will shortly replace $\rho(\omega)$ by $\chi(\omega)$ which, as we've just seen, has no poles in the upper half plane). We can define a new function $f(\omega)$ by the integral,

$$f(\omega) = \frac{1}{i\pi} \int_a^b \frac{\rho(\omega')}{\omega' - \omega} d\omega' \quad (4.8)$$

Here the integral is taken along the interval $\omega' \in [a, b]$ of the real line. However, when ω also lies in this interval, we have a problem because the integral diverges at $\omega' = \omega$. To avoid this, we can simply deform the contour of the integral into the complex plane, either running just above the singularity along $\omega' + i\epsilon$ or just below the singularity along $\omega' - i\epsilon$. Alternatively (in fact, equivalently) we could just shift the position of the singularity to $\omega \rightarrow \omega \mp \epsilon$. In both cases we just skim by the singularity and the integral is well defined. The only problem is that we get different answers depending on which way we do things. Indeed, the difference between the two answers is given by Cauchy's residue theorem,

$$\frac{1}{2}[f(\omega + i\epsilon) - f(\omega - i\epsilon)] = \rho(\omega) \quad (4.9)$$

The difference between $f(\omega + i\epsilon)$ and $f(\omega - i\epsilon)$ means that the function $f(\omega)$ is discontinuous across the real axis for $\omega \in [a, b]$. If $\rho(\omega)$ is everywhere analytic, this discontinuity is a branch cut.

We can also define the average of the two functions either side of the discontinuity. This is usually called the *principal value*, and is denoted by adding the symbol \mathcal{P} before the integral,

$$\frac{1}{2}[f(\omega + i\epsilon) + f(\omega - i\epsilon)] \equiv \frac{1}{i\pi} \mathcal{P} \int_a^b \frac{\rho(\omega')}{\omega' - \omega} d\omega' \quad (4.10)$$

We can get a better handle on the meaning of this principal part if we look at the real and imaginary pieces of the denominator in the integrand $1/[\omega' - (\omega \pm i\epsilon)]$,

$$\frac{1}{\omega' - (\omega \pm i\epsilon)} = \frac{\omega' - \omega}{(\omega' - \omega)^2 + \epsilon^2} \pm \frac{i\epsilon}{(\omega' - \omega)^2 + \epsilon^2} \quad (4.11)$$

By taking the sum of $f(\omega + i\epsilon)$ and $f(\omega - i\epsilon)$ in (4.10), we isolate the real part, the first term in (4.11). This is shown in the left-hand figure. It can be thought of as a suitably cut-off version of $1/(\omega' - \omega)$. It's as if we have deleted a small segment of this function lying symmetrically about divergent point ω and replaced it with a smooth function going through zero. This is the usual definition of the principal part of an integral.

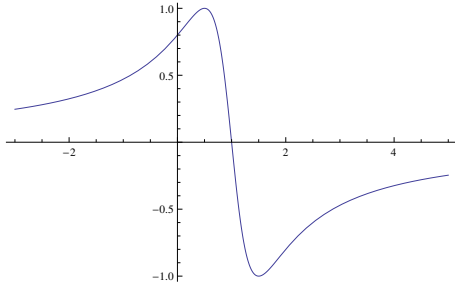


Figure 9: The real part of the function (4.11), plotted with $\omega' = 1$ and $\epsilon = 0.5$.

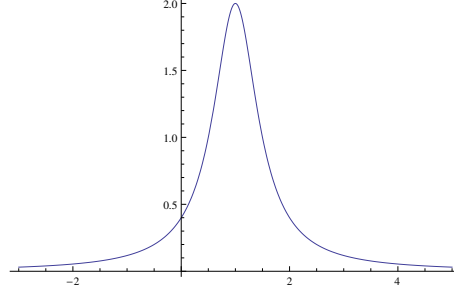


Figure 10: The imaginary part of the function (4.11), plotted with $\omega' = 1$ and $\epsilon = 0.5$

We can also see the meaning of the imaginary part of $1/(\omega' - \omega)$, the second term in (4.11). This is shown in the right-hand figure. As $\epsilon \rightarrow 0$, it tends towards a delta function, as expected from (4.9). For finite ϵ , it is a regularized version of the delta function.

Kramers-Kronig

Let's now apply this discussion to our response function $\chi(\omega)$. We'll be interested in the integral

$$\frac{1}{i\pi} \oint_C d\omega' \frac{\chi(\omega')}{\omega' - \omega} \quad \omega \in \mathbf{R} \quad (4.12)$$

where the contour C skims just above the real axis, before closing at infinity in the upper-half plane. We'll need to make one additional assumption: that $\chi(z)$ falls off faster than $1/|z|$ at infinity. If this holds, the integral is the same as we consider in (4.8) with $[a, b] \rightarrow [-\infty, +\infty]$. Indeed, in the language of the previous discussion, the integral is $f(\omega - i\epsilon)$, with $\rho = \chi$.

We apply the formulae (4.9) and (4.10). It gives

$$f(\omega - i\epsilon) = \frac{1}{i\pi} \mathcal{P} \left[\int_{-\infty}^{+\infty} d\omega' \frac{\chi(\omega')}{\omega' - \omega} \right] - \chi(\omega)$$

But we know the integral in (4.12) has to be zero since $\chi(\omega)$ has no poles in the upper-half plane. This means that $f(\omega - i\epsilon) = 0$, or

$$\chi(\omega) = \frac{1}{i\pi} \mathcal{P} \int_{-\infty}^{+\infty} d\omega' \frac{\chi(\omega')}{\omega' - \omega} \quad (4.13)$$

The important part for us is that factor of “ i ” sitting in the denominator. Taking real and imaginary parts, we learn that

$$\operatorname{Re} \chi(\omega) = \mathcal{P} \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\operatorname{Im} \chi(\omega')}{\omega' - \omega} \quad (4.14)$$

and

$$\operatorname{Im} \chi(\omega) = -\mathcal{P} \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\operatorname{Re} \chi(\omega')}{\omega' - \omega} \quad (4.15)$$

These are the *Kramers-Kronig* relations. They follow from causality alone and tell us that the dissipative, imaginary part of the response function $\chi''(\omega)$ is determined in terms of the reactive, real part, $\chi'(\omega)$ and vice-versa. However, the relationship is not local in frequency space: you need to know $\chi'(\omega)$ for all frequencies in order to reconstruct χ'' for any single frequency.

There’s another way of writing these relations which is also useful and tells us how we can reconstruct the full response function $\chi(\omega)$ if we only know the dissipative part. To see this, look at

$$\int_{-\infty}^{+\infty} \frac{d\omega'}{i\pi} \frac{\operatorname{Im} \chi(\omega')}{\omega' - \omega - i\epsilon} \quad (4.16)$$

where the $-i\epsilon$ in the denominator tells us that this is an integral just below the real axis. Again using the formulae (4.9) and (4.10), we have

$$\begin{aligned} \int_{-\infty}^{+\infty} \frac{d\omega'}{i\pi} \frac{\operatorname{Im} \chi(\omega')}{\omega' - \omega - i\epsilon} &= \operatorname{Im} \chi(\omega) + \mathcal{P} \int_{-\infty}^{+\infty} \frac{d\omega'}{i\pi} \frac{\operatorname{Im} \chi(\omega')}{\omega' - \omega - i\epsilon} \\ &= \operatorname{Im} \chi(\omega) - i \operatorname{Re} \chi(\omega) \end{aligned} \quad (4.17)$$

Or, rewriting as $\chi(\omega) = \operatorname{Re} \chi(\omega) + i \operatorname{Im} \chi(\omega)$, we get

$$\chi(\omega) = \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\operatorname{Im} \chi(\omega')}{\omega' - \omega - i\epsilon} \quad (4.18)$$

If you know the dissipative part of the response function, you know everything.

An Application: Susceptibility

Suppose that turning on a perturbation ϕ induces a response $\langle \mathcal{O} \rangle$ for some observable of our system. Then the *susceptibility* is defined as

$$\chi = \left. \frac{\partial \langle \mathcal{O} \rangle}{\partial \phi} \right|_{\omega=0}$$

We've called the susceptibility χ which is the same name that we gave to the response function. And, indeed, from the definition of linear response (4.4), the former is simply the zero frequency limit of the latter:

$$\chi = \lim_{\omega \rightarrow 0} \chi(\omega)$$

A common example, which we met in our first course in statistical mechanics, is the change of magnetization M of a system in response to an external magnetic field B . The aptly named magnetic susceptibility is given by $\chi = \partial M / \partial B$.

From (4.18), we can write the susceptibility as

$$\chi = \int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\text{Im}\chi(\omega')}{\omega' - i\epsilon} \quad (4.19)$$

We see that if you can do an experiment to determine how much the system absorbs at all frequencies, then from this information you can determine the response of the system at zero frequency. This is known as the thermodynamic sum rule.

4.2 Classical Examples

The definitions and manipulations of the previous section can appear somewhat abstract the first time you encounter them. Some simple examples should shed some light. The main example we'll focus on is the same one that accompanies us through most of physics: the classical harmonic oscillator.

4.2.1 The Damped Harmonic Oscillator

The equation of motion governing the damped harmonic oscillator in the presence of a driving force is

$$\ddot{x} + \gamma\dot{x} + \omega_0^2 x = F(t) \quad (4.20)$$

Here γ is the friction. We denote the undamped frequency as ω_0 , saving ω for the frequency of the driving force as in the previous section.. We want to determine the response function, or Green's function, $\chi(t - t')$ of this system. This is the function which effectively solves the dynamics for us, meaning that if someone tells us the driving force $F(t)$, the motion is given by

$$x(t) = \int_{-\infty}^{+\infty} dt' \chi(t - t') F(t') \quad (4.21)$$

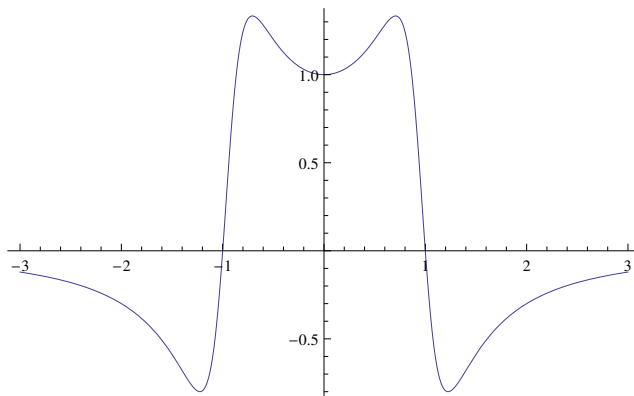


Figure 11: The real, reactive part of the response function for the underdamped harmonic oscillator, plotted with $\omega_0 = 1$ and $\gamma = 0.5$.

There is a standard method to figure out $\chi(t)$. Firstly, we introduce the (inverse) Fourier transform

$$\chi(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \chi(\omega)$$

We plug this into the equation of motion (4.20) to get

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{+\infty} dt' [-\omega^2 - i\gamma\omega + \omega_0^2] e^{-i\omega(t-t')} \chi(\omega) F(t') = F(t)$$

which is solved if the $\int d\omega$ gives a delta function. But since we can write a delta function as $2\pi\delta(t) = \int d\omega e^{-i\omega t}$, that can be achieved by simply taking

$$\chi(\omega) = \frac{1}{-\omega^2 + i\gamma\omega + \omega_0^2} \quad (4.22)$$

There's a whole lot of simple physics sitting in this equation which we'll now take some time to extract. All the lessons that we'll learn carry over to more complicated systems.

Firstly, we can look at the *susceptibility*, meaning $\chi(\omega = 0) = 1/\omega_0^2$. This tells us how much the observable changes by a perturbation of the system, i.e. a static force: $x = F/\omega_0^2$ as expected.

Let's look at the structure of the response function on the complex ω -plane. The poles sit at $\omega_*^2 + i\gamma\omega_* - \omega_0^2 = 0$ or, solving the quadratic, at

$$\omega_* = -\frac{i\gamma}{2} \pm \sqrt{\omega_0^2 - \gamma^2/4}$$

There are two different regimes that we should consider separately,

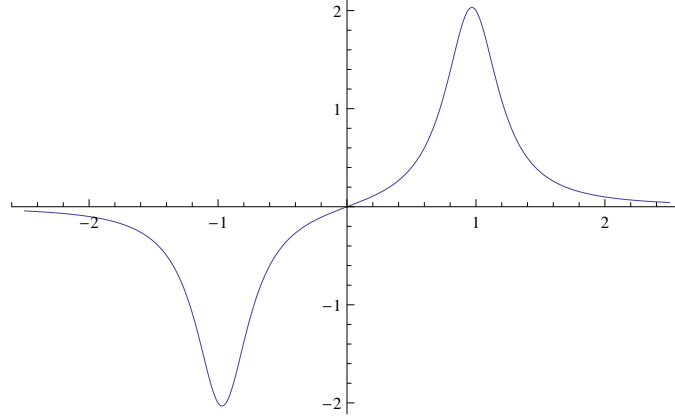


Figure 12: The imaginary, dissipative part of the response function for the underdamped harmonic oscillator, plotted with $\omega_0 = 1$ and $\gamma = 0.5$.

- **Underdamped:** $\omega_0^2 > \gamma^2/4$. In this case, the poles have both a real and imaginary part. They both sit on the lower half plane. This is in agreement with our general lesson of causality which tells us that the response function must be analytic in the upper-half plane
- **Overdamped:** $\omega_0^2 < \gamma^2/4$. Now the poles lie on the negative imaginary axis. Again, there are none in the upper-half place, consistent with causality.

We can gain some intuition by plotting the real and imaginary part of the response function for $\omega \in \mathbf{R}$. Firstly, the real part is shown in Figure 11 where we plot

$$\text{Re}\chi(\omega) = \frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (4.23)$$

This is the reactive part. The higher the function, the more the system will respond to a given frequency. Notice that $\text{Re}\chi(\omega)$ is an even function, as expected.

More interesting is the dissipative part of the response function,

$$\text{Im}\chi(\omega) = \frac{\omega\gamma}{(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2} \quad (4.24)$$

This is an odd function. In the underdamped case, this is plotted in Figure 12. Notice that $\text{Im}\chi$ is proportional to γ , the coefficient of friction. The function peaks around $\pm\omega_0$, at frequencies where the system naturally vibrates. This is because this is where the system is able to absorb energy. However, as $\gamma \rightarrow 0$, the imaginary part doesn't become zero: instead it tends towards two delta functions situated at $\pm\omega_0$.

4.2.2 Dissipation

We can see directly how $\text{Im}\chi(\omega)$ is related to dissipation by computing the energy absorbed by the system. This what we used to call the work done on the system before we became all sophisticated and grown-up. It is

$$\begin{aligned}
\frac{dW}{dt} &= F(t)\dot{x}(t) \\
&= F(t)\frac{d}{dt}\int_{-\infty}^{+\infty} dt' \chi(t-t')F(t') \\
&= F(t)\int_{-\infty}^{+\infty} dt' \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} (-i\omega)e^{-i\omega(t-t')} \chi(\omega)F(t') \\
&= \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{d\omega'}{2\pi} [-i\omega\chi(\omega)]e^{-i(\omega+\omega')t} F(\omega)F(\omega')
\end{aligned} \tag{4.25}$$

Let's drive the system with a force of a specific frequency Ω , so that

$$F(t) = F_0 \cos \Omega t = F_0 \text{Re}(e^{-i\Omega t})$$

Notice that it's crucial to make sure that the force is real at this stage of the calculation because the reality of the force (or source) was the starting point for our discussion of the analytic properties of response functions in section 4.1.2. In a more pedestrian fashion, we can see that it's going to be important because our equation above is not linear in $F(\omega)$, so it's necessary to take the real part before progressing. Taking the Fourier transform, the driving force is

$$F(\omega) = 2\pi F_0 [\delta(\omega - \Omega) + \delta(\omega + \Omega)]$$

Inserting this into (4.25) gives

$$\frac{dW}{dt} = -iF_0^2\Omega [\chi(\Omega)e^{-i\Omega t} - \chi(-\Omega)e^{+i\Omega t}] [e^{-i\Omega t} + e^{i\Omega t}] \tag{4.26}$$

This is still oscillating with time. It's more useful to take an average over a cycle,

$$\overline{\frac{dW}{dt}} \equiv \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \frac{dW}{dt} = -iF_0^2\Omega [\chi(\Omega) - \chi(-\Omega)]$$

But we've already seen that $\text{Re}\chi(\omega)$ is an even function, while $\text{Im}\chi(\omega)$ is an odd function. This allows us to write

$$\overline{\frac{dW}{dt}} = 2F_0^2\Omega \text{Im}\chi(\Omega) \tag{4.27}$$

We see that the work done is proportional to $\text{Im}\chi$. To derive this result, we didn't need the exact form of the response function; only the even/odd property of the real/imaginary parts, which follow on general grounds. For our damped harmonic oscillator, we can now use the explicit form (4.24) to derive

$$\frac{\overline{dW}}{dt} = 2F_0^2 \frac{\gamma\Omega^2}{(\omega_0^2 - \Omega^2)^2 + (\gamma\Omega)^2}$$

This is a maximum when we shake the harmonic oscillator at its natural frequency, $\Omega = \omega_0$. As this example illustrates, the imaginary part of the response function tells us the frequencies at which the system naturally vibrates. These are the frequencies where the system can absorb energy when shaken.

4.2.3 Hydrodynamic Response

For our final classical example, we'll briefly return to the topic of hydrodynamics. One difference with our present discussion is that the dynamical variables are now functions of both space and time. A typical example that we'll focus on here is the mass density, $\rho(\vec{x}, t)$. Similarly, the driving force (or, in the context of quantum mechanics, the source) is similarly a function of space and time.

Rather than playing at the full Navier-Stokes equation, here we'll instead just look at a simple model of diffusion. The continuity equation is

$$\frac{\partial\rho}{\partial t} + \vec{\nabla} \cdot \vec{J} = 0$$

We'll write down a simple model for the current,

$$\vec{J} = -D\vec{\nabla}\rho + \vec{F} \tag{4.28}$$

where D is the diffusion constant and the first term gives rise to Fick's law that we met already in Section 1. The second term, $\vec{F} = \vec{F}(\vec{x}, t)$, is the driving force. . Combining this with the continuity equation gives,

$$\frac{\partial\rho}{\partial t} - D\nabla^2\rho = -\vec{\nabla} \cdot \vec{F} \tag{4.29}$$

We want to understand the response functions associated to this force. This includes both the response of ρ and the response of \vec{J} ,

For simplicity, let's work in a single spatial dimension so that we can drop the vector indices. We write

$$\begin{aligned}\rho(x, t) &= \int dx' dt' \chi_{\rho J}(x', t'; x, t) F(x', t) \\ J(x, t) &= \int dx' dt' \chi_{JJ}(x', t'; x, t) F(x', t)\end{aligned}$$

where we've called the second label J on both of these functions to reflect the fact that F is a driving force for J . We follow our discussion of Section 4.1.1. We now assume that our system is invariant under both time and space translations which ensures that the response function depend only on $t' - t$ and $x' - x$. We then Fourier transform with respect to both time and space. For example,

$$\rho(\omega, k) = \int dx dt e^{i(\omega t - kx)} \rho(x, t)$$

Then in momentum and frequency space, the response functions become

$$\begin{aligned}\rho(\omega, k) &= \chi_{\rho J}(\omega, k) F(\omega, k) \\ J(\omega, k) &= \chi_{JJ}(\omega, k) F(\omega, k)\end{aligned}$$

The diffusion equation (4.29) immediately gives an expression for $\chi_{\rho J}$. Substituting the resulting expression into (4.28) then gives us χ_{JJ} . The response functions are

$$\chi_{\rho J} = \frac{ik}{-i\omega + Dk^2} \quad , \quad \chi_{JJ} = \frac{-i\omega}{-i\omega + Dk^2}$$

Both of the denominator have poles on the imaginary axis at $\omega = -iDk^2$. This is the characteristic behaviour of response functions capturing diffusion.

Our study of hydrodynamics in Sections 2.4 and 2.5 revealed a different method of transport, namely sound. For the ideal fluid of Section 2.4, the sound waves travelled without dissipation. The associated response function has the form

$$\chi_{\text{sound}} \sim \frac{1}{\omega^2 - v_s^2 k^2}$$

which is simply the Green's function for the wave equation. If one includes the effect of dissipation, the poles of the response function pick up a (negative) imaginary part. For sound waves in the Navier-Stokes equation, we computed the location of these poles in (2.76).

4.3 Quantum Mechanics and the Kubo Formula

Let's now return to quantum mechanics. Recall the basic set up: working in the Heisenberg picture, we add to a Hamiltonian the perturbation

$$H_{\text{source}}(t) = \phi_j(t)\mathcal{O}_j(t) \quad (4.30)$$

where there is an implicit sum over j , labelling the operators in the theory and, correspondingly, the different sources that we can turn on. Usually in any given situation we only turn on a source for a single operator, but we may be interested in how this source affects the expectation value of any other operator in the theory, $\langle \mathcal{O}_i \rangle$. However, if we restrict to small values of the source, we can address this using standard perturbation theory. We introduce the time evolution operator,

$$U(t, t_0) = T \exp \left(-i \int_{t_0}^t H_{\text{source}}(t') dt' \right)$$

which is constructed to obey the operator equation $idU/dt = H_{\text{source}}U$. Then, switching to the interaction picture, states evolve as

$$|\psi(t)\rangle_I = U(t, t_0)|\psi(t_0)\rangle_I$$

We'll usually be working in an ensemble of states described by a density matrix ρ . If, in the distant past $t \rightarrow -\infty$, the density matrix is given by ρ_0 , then at some finite time it evolves as

$$\rho(t) = U(t)\rho_0U^{-1}(t)$$

with $U(t) = U(t, t_0 \rightarrow -\infty)$. From this we can compute the expectation value of any operator \mathcal{O}_j in the presence of the sources ϕ . Working to first order in perturbation theory (from the third line below), we have

$$\begin{aligned} \langle \mathcal{O}_i(t) \rangle|_{\phi} &= \text{Tr } \rho(t)\mathcal{O}_i(t) \\ &= \text{Tr } \rho_0(t)U^{-1}(t)\mathcal{O}_i(t)U(t) \\ &\approx \text{Tr } \rho_0(t) \left(\mathcal{O}_i(t) + i \int_{-\infty}^t dt' [H_{\text{source}}(t'), \mathcal{O}_i(t)] + \dots \right) \\ &= \langle \mathcal{O}_i(t) \rangle|_{\phi=0} + i \int_{-\infty}^t dt' \langle [H_{\text{source}}(t'), \mathcal{O}_i(t)] \rangle + \dots \end{aligned}$$

Inserting our explicit expression for the source Hamiltonian gives the change in the expectation value, $\delta\langle \mathcal{O}_i \rangle = \langle \mathcal{O}_i \rangle_{\phi} - \langle \mathcal{O}_i \rangle_{\phi=0}$,

$$\begin{aligned} \delta\langle \mathcal{O}_i \rangle &= i \int_{-\infty}^t dt' \langle [\mathcal{O}_j(t'), \mathcal{O}_i(t)] \rangle \phi_j(t') \\ &= i \int_{-\infty}^{+\infty} dt' \theta(t-t') \langle [\mathcal{O}_j(t'), \mathcal{O}_i(t)] \rangle \phi_j(t') \end{aligned} \quad (4.31)$$

where, in the second line, we have done nothing more than use the step function to extend the range of the time integration to $+\infty$. Comparing this to our initial definition given in (4.4), we see that the response function in a quantum theory is given by the two-point function,

$$\chi_{ij}(t-t') = -i\theta(t-t') \langle [\mathcal{O}_i(t), \mathcal{O}_j(t')] \rangle \quad (4.32)$$

This important result is known as the *Kubo formula*. (Although sometimes the name “Kubo formula” is restricted to specific examples of this equation which govern transport properties in quantum field theory. We will derive these examples in Section 4.4).

4.3.1 Dissipation Again

Before we make use of the Kubo formula, we will first return to the question of dissipation. Here we repeat the calculation of 4.2.2 where we showed that, for classical systems, the energy absorbed by a system is proportional to $\text{Im } \chi$. Here we do the same for quantum systems. The calculation is a little tedious, but worth ploughing through.

As in the classical context, the work done is associated to the change in the energy of the system which, this time, can be written as

$$\frac{dW}{dt} = \frac{d}{dt} \text{Tr } \rho H = \text{Tr}(\rho \dot{H} + \dot{\rho} H)$$

To compute physical observables, it doesn’t matter if we work in the Heisenberg or Schrödinger picture. So let’s revert momentarily back to the Schrödinger picture. Here, the density matrix evolves as $i\dot{\rho} = [H, \rho]$, so the first term above vanishes. Meanwhile, the Hamiltonian H changes because we’re sitting there playing around with the source (4.30), providing an explicit time dependence. To simplify our life, we’ll assume that we turn on just a single source, ϕ . Then, in the Schrödinger picture

$$\dot{H} = \mathcal{O}\dot{\phi}(t)$$

This gives us the energy lost by the system,

$$\frac{dW}{dt} = \text{Tr}(\rho \mathcal{O} \dot{\phi}) = \langle \mathcal{O} \rangle_{\phi} \dot{\phi} = [\langle \mathcal{O} \rangle_{\phi=0} + \delta \langle \mathcal{O} \rangle] \dot{\phi}$$

We again look at a periodically varying source which we write as

$$\phi(t) = \text{Re}(\phi_0 e^{-i\Omega t})$$

and we again compute the average work done over a complete cycle

$$\frac{\overline{dW}}{dt} = \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \frac{dW}{dt}$$

The term $\langle \mathcal{O}(\vec{x}) \rangle_0$ cancels out when integrated over the full cycle. This leaves us with

$$\begin{aligned}
\frac{\overline{dW}}{dt} &= \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \int_{-\infty}^{+\infty} dt' \chi(t-t') \phi(t') \dot{\phi}(t) \\
&= \frac{\Omega}{2\pi} \int_0^{2\pi/\Omega} dt \int_{-\infty}^{+\infty} dt' \int \frac{d\omega}{2\pi} \chi(\omega) e^{-i\omega(t-t')} \\
&\quad \times \frac{1}{4} \left[\phi_0 e^{-i\Omega t'} + \phi_0^* e^{+i\Omega t'} \right] \left[-i\Omega \phi_0 e^{-i\Omega t} + i\Omega \phi_0^* e^{+i\Omega t} \right] \\
&= \frac{1}{4} [\chi(\Omega) - \chi(-\Omega)] |\phi_0|^2 i\Omega
\end{aligned}$$

where the ϕ^2 and ϕ^{*2} terms have canceled out after performing the $\int dt$. Continuing, we only need the fact that the real part of χ is even while the imaginary part is odd. This gives us the result

$$\frac{\overline{dW}}{dt} = \frac{1}{2} \Omega \chi''(\Omega) |\phi_0|^2 \quad (4.33)$$

Finally, this calculation tells us about another property of the response function. If we perform work on a system, the energy should increase. This translates into a positivity requirement $\Omega \chi''(\Omega) \geq 0$. More generally, the requirement is that $\Omega \chi''_{ij}(\Omega)$ is a positive definite matrix.

Spectral Representation

In the case of the damped harmonic oscillator, we saw explicitly that the dissipation was proportional to the coefficient of friction, γ . But for our quantum systems, the dynamics is entirely Hamiltonian: there is no friction. So what is giving rise to the dissipation? In fact, the answer to this can also be found in our analysis of the harmonic oscillator, for there we found that in the limit $\gamma \rightarrow 0$, the dissipative part of the response function χ'' doesn't vanish but instead reduces to a pair of delta functions. Here we will show that a similar property holds for a general quantum system.

We'll take the state of our quantum system to be described by a density matrix describing the canonical ensemble, $\rho = e^{-\beta H}$. Taking the Fourier transform of the Kubo formula (4.32) gives

$$\chi_{ij}(\omega) = -i \int_0^\infty dt e^{i\omega t} \text{Tr} \left(e^{-\beta H} [\mathcal{O}_i(t), \mathcal{O}_j(0)] \right)$$

We will need to use the fact that operators evolve as $\mathcal{O}_i(t) = U^{-1} \mathcal{O}_i(0) U$ with $U = e^{-iHt}$ and will evaluate $\chi_{ij}(\omega)$ by inserting complete basis of energy states

$$\chi_{ij}(\omega) = -i \int_0^\infty dt e^{i\omega t} \sum_{mn} e^{-E_m \beta} [\langle m | \mathcal{O}_i | n \rangle \langle n | \mathcal{O}_j | m \rangle e^{i(E_m - E_n)t}]$$

$$-\langle m|\mathcal{O}_j|n\rangle\langle n|\mathcal{O}_i|m\rangle e^{i(E_n-E_m)t}$$

To ensure that the integral is convergent for $t > 0$, we replace $\omega \rightarrow \omega + i\epsilon$. Then performing the integral over $\int dt$ gives

$$\begin{aligned}\chi_{ij}(\omega + i\epsilon) &= \sum_{m,n} e^{-E_m\beta} \left[\frac{(\mathcal{O}_i)_{mn}(\mathcal{O}_j)_{nm}}{\omega + E_m - E_n + i\epsilon} - \frac{(\mathcal{O}_j)_{mn}(\mathcal{O}_i)_{nm}}{\omega + E_n - E_m + i\epsilon} \right] \\ &= \sum_{m,n} \frac{(\mathcal{O}_i)_{mn}(\mathcal{O}_j)_{nm}}{\omega + E_m - E_n + i\epsilon} (e^{-E_m\beta} - e^{-E_n\beta})\end{aligned}$$

which tells us that the response function has poles just below the real axis,

$$\omega = E_n - E_m - i\epsilon$$

Of course, we knew on general grounds that the poles couldn't lie in the upper half-plane: we see that in a Hamiltonian system the poles lie essentially on the real axis (as $\epsilon \rightarrow 0$) at the values of the frequency that can excite the system from one energy level to another. In any finite quantum system, we have an isolated number of singularities.

As in the case of the harmonic oscillator, in the limit $\epsilon \rightarrow 0$, the imaginary part of the response function doesn't disappear: instead it becomes a sum of delta function spikes

$$\chi'' \sim \sum_{m,n} \frac{\epsilon}{(\omega + E_m - E_n)^2 + \epsilon^2} \longrightarrow \sum_{m,n} \delta(\omega - (E_n - E_m))$$

The expression above is appropriate for quantum systems with discrete energy levels. However, in infinite systems — and, in particular, in the quantum field theories that we turn to shortly — these spikes can merge into smooth functions and dissipative behaviour can occur for all values of the frequency.

4.3.2 Fluctuation-Dissipation Theorem

We have seen above that the imaginary part of the response function governs the dissipation in a system. Yet, the Kubo formula (4.32) tells us that the response formula can be written in terms of a two-point correlation function in the quantum theory. And we know that such two-point functions provide a measure of the variance, or fluctuations, in the system. This is the essence of the fluctuation-dissipation theorem which we'll now make more precise.

First, the form of the correlation function in (4.32) — with the commutator and funny theta term — isn't the simplest kind of correlation we could image. The more basic correlation function is simply

$$S_{ij}(t) \equiv \langle \mathcal{O}_i(t) \mathcal{O}_j(0) \rangle$$

where we have used time translational invariance to set the time at which \mathcal{O}_j is evaluated to zero. The Fourier transform of this correlation function is

$$S_{ij}(\omega) = \int dt e^{i\omega t} S_{ij}(t) \quad (4.34)$$

The content of the fluctuation-dissipation theorem is to relate the dissipative part of the response function to the fluctuations $S(\omega)$ in the vacuum state which, at finite temperature, means the canonical ensemble $\rho = e^{-\beta H}$.

There is a fairly pedestrian proof of the theorem using spectral decomposition (i.e. inserting a complete basis of energy eigenstates as we did in the previous section). Here we instead give a somewhat slicker proof although, as we will see, it requires us to do something fishy somewhere. We proceed by writing an expression for the dissipative part of the response function using the Kubo formula (4.32),

$$\begin{aligned} \chi''_{ij}(t) &= -\frac{i}{2} [\chi_{ij}(t) - \chi_{ji}(-t)] \\ &= -\frac{1}{2} \theta(t) \left[\langle \mathcal{O}_i(t) \mathcal{O}_j(0) \rangle - \langle \mathcal{O}_j(0) \mathcal{O}_i(t) \rangle \right] \\ &\quad + \frac{1}{2} \theta(-t) \left[\langle \mathcal{O}_j(-t) \mathcal{O}_i(0) \rangle - \langle \mathcal{O}_i(0) \mathcal{O}_j(-t) \rangle \right] \end{aligned}$$

By time translational invariance, we know that $\langle \mathcal{O}_j(0) \mathcal{O}_i(t) \rangle = \langle \mathcal{O}_j(-t) \mathcal{O}_i(0) \rangle$. This means that the step functions arrange themselves to give $\theta(t) + \theta(-t) = 1$, leaving

$$\chi''_{ij}(t) = -\frac{1}{2} \langle \mathcal{O}_i(t) \mathcal{O}_j(0) \rangle + \frac{1}{2} \langle \mathcal{O}_j(-t) \mathcal{O}_i(0) \rangle \quad (4.35)$$

But we can re-order the operators in the last term. To do this, we need to be sitting in the canonical ensemble, so that the expectation value is computed with respect to the Boltzmann density matrix. We then have

$$\begin{aligned} \langle \mathcal{O}_j(-t) \mathcal{O}_i(0) \rangle &= \text{Tr} e^{-\beta H} \mathcal{O}_j(-t) \mathcal{O}_i(0) \\ &= \text{Tr} e^{-\beta H} \mathcal{O}_j(-t) e^{\beta H} e^{-\beta H} \mathcal{O}_i(0) \\ &= \text{Tr} e^{-\beta H} \mathcal{O}_i(0) \mathcal{O}_j(-t + i\beta) \\ &= \langle \mathcal{O}_i(t - i\beta) \mathcal{O}_j(0) \rangle \end{aligned}$$

The third line above is where we've done something slippery: we've treated the density matrix $\rho = e^{-\beta H}$ as a time evolution operator, but one which evolves the operator in the imaginary time direction! In the final line we've used time translational invariance, now both in real and imaginary time directions. While this may look dodgy, we can turn it into something more palatable by taking the Fourier transform. The dissipative part of the response function can be written in terms of correlation functions as

$$\chi''_{ij}(t) = -\frac{1}{2} \left[\langle \mathcal{O}_i(t) \mathcal{O}_j(0) \rangle - \langle \mathcal{O}_i(t - i\beta) \mathcal{O}_j(0) \rangle \right] \quad (4.36)$$

Taking the Fourier transform then gives us our final expression:

$$\chi''_{ij}(\omega) = -\frac{1}{2} [1 - e^{-\beta\omega}] S_{ij}(\omega) \quad (4.37)$$

This is the fluctuation-dissipation theorem, relating the fluctuations in frequency space, captured by $S(\omega)$, to the dissipation, captured by $\chi''(\omega)$. Indeed, a similar relationship holds already in classical physics; the most famous example is the Einstein relation that we met in Section 3.1.3.

The physics behind (4.37) is highlighted a little better if we invert the equation. We can write

$$S_{ij}(\omega) = -2[n_B(\omega) + 1] \chi''_{ij}(\omega)$$

where $n_B(\omega) = (e^{\beta\omega} - 1)^{-1}$ is the Bose-Einstein distribution function. Here we see explicitly the two contributions to the fluctuations: the $n_B(\omega)$ factor is due to thermal effects; the “+1” can be thought of as due to inherently quantum fluctuations. As usual, the classical limit occurs for high temperatures with $\beta\omega \ll 1$ where $n_B(\omega) \approx k_B T / \omega$. In this regime, the fluctuation dissipation theorem reduces to its classical counterpart

$$S_{ij}(\omega) = -\frac{2k_B T}{\omega} \chi''_{ij}(\omega)$$

4.4 Response in Quantum Field Theory

We end these lectures by describing how response theory can be used to compute some of the transport properties that we've encountered in previous sections. To do this, we work with quantum field theory¹⁰, where the operators become functions of space and time, $\mathcal{O}(\vec{x}, t)$. In the context of condensed matter, this is the right framework to describe many-body physics. In the context of particle physics, this is the right framework to describe everything.

¹⁰See <http://www.damtp.cam.ac.uk/user/tong/qft.html> for an introductory course on quantum field theory.

Suppose that you take a quantum field theory, place it in a state with a finite amount of stuff (whatever that stuff is) and heat it up. What is the right description of the resulting dynamics? From our earlier discussion, we know the answer: the low-energy excitations of the system are described by hydrodynamics, simply because this is the universal description that applies to everything. (Actually, we're brushing over something here: the exact form of the hydrodynamics depends on the symmetries of the theory, both broken and unbroken). All that remains is to identify the transport coefficients, such as viscosity and thermal conductivity, that arise in the hydrodynamic equations. But how to do that starting from the quantum field?

The answer to this question lies in the machinery of linear response that we developed above. For a quantum field, we again add source terms to the action, now of the form

$$H_{\text{source}}(t) = \int d^{d-1}\vec{x} \phi_i(\vec{x}, t) \mathcal{O}_i(\vec{x}, t) \quad (4.38)$$

The response function χ is again defined to be the change of the expectation values of \mathcal{O} in the presence of the source ϕ ,

$$\delta\langle\mathcal{O}_i(\vec{x}, t)\rangle = \int d^d\vec{x}' dt' \chi_{ij}(\vec{x}, t; \vec{x}', t') \phi_j(\vec{x}', t') \quad (4.39)$$

All the properties of the response function that we derived previously also hold in the context of quantum field theory. Indeed, for the most part, the label \vec{x} and \vec{x}' can be treated in the same way as the label i, j . Going through the steps leading to the Kubo formula (4.32), we now find

$$\chi_{ij}(\vec{x}, \vec{x}'; t - t') = -i\theta(t - t')\langle[\mathcal{O}_i(\vec{x}, t), \mathcal{O}_j(\vec{x}', t')]\rangle \quad (4.40)$$

If you've taken a first course on quantum field theory, then you know that the two-point functions are Green's functions. Usually, when thinking about scattering amplitudes, we work with time-ordered (Feynman) correlation functions that are relevant for building perturbation theory. Here, we're interested in the *retarded* correlation functions, characterised by the presence of the step function sitting in front of (4.40).

Finally, if the system exhibits translational invariance in both space and time, then the response function depends only on the differences $t - t'$ and $\vec{x} - \vec{x}'$. In this situation it is useful to work in momentum and frequency space, so that the (4.39) becomes

$$\delta\langle\mathcal{O}_i(\vec{k}, \omega)\rangle = \chi_{ij}(\vec{k}, \omega) \phi_j(\vec{k}, \omega) \quad (4.41)$$

Electrical Conductivity

Consider a quantum field theory with a $U(1)$ global symmetry. By Noether's theorem, there is an associated conserved current $J^\mu = (J^0, J^i)$, obeying $\partial_\mu J^\mu = 0$. This current is an example of a composite operator. It couples to a source which is a gauge field $A_\mu(x)$,

$$H_{\text{source}} = \int d^{d-1}\vec{x} A_\mu J^\mu \quad (4.42)$$

Here A_μ is the background gauge field of electromagnetism. However, for the purposes of our discussion, we do not take A_μ to have dynamics of its own. Instead, we treat it as a fixed source, under our control.

There is, however, a slight subtlety. In the presence of the background gauge field, the current itself may be altered so that it depends on A_μ . A simple, well known, example of this occurs for a free, relativistic, complex scalar field φ . The conserved current in the presence of the background field is given by

$$J^\mu = ie[\varphi^\dagger \partial^\mu \varphi - (\partial^\mu \varphi^\dagger)\varphi] - e^2 A^\mu \varphi^\dagger \varphi \quad (4.43)$$

where e is the electric charge. With this definition, the Lagrangian can be written in terms of covariant derivatives $\mathcal{D}_\mu \varphi = \partial_\mu \varphi - ieA_\mu \varphi$,

$$L = \int d^{d-1}\vec{x} |\partial_\mu \varphi|^2 + A_\mu J^\mu = \int d^{d-1}\vec{x} |\mathcal{D}_\mu \varphi|^2 \quad (4.44)$$

For non-relativistic fields (either bosons or fermions), similar A_μ terms arise in the current for the spatial components.

We want to derive the response of the system to a background electric field. Which, in more basic language, means that we want to derive Ohm's law in our quantum field theory. This is

$$\langle J_i(\vec{k}, \omega) \rangle = \sigma_{ij}(\vec{k}, \omega) E_j(\vec{k}, \omega) \quad (4.45)$$

Here E_i is the background electric field in Fourier space and σ_{ij} is the conductivity tensor. In a system with rotational and parity invariance (which, typically means in the absence of a magnetic field) we have $\sigma_{ij} = \sigma \delta_{ij}$, so that the current is parallel to the applied electric field. Here we will work with the more general case. Our goal is to get an expression for σ_{ij} in terms of correlation functions in the field theory. Applying (4.41) with the perturbation (4.42), we have

$$\delta \langle J_\mu \rangle = \langle J_\mu \rangle - \langle J_\mu \rangle_0 = -i \int_{-\infty}^t dt' d^3\vec{x}' \langle [J_\mu(\vec{x}, t), J_\nu(\vec{x}', t')] \rangle_0 A_\nu(\vec{x}', t') \quad (4.46)$$