8.512 Theory of Solids II
Spring 2009

Lecture 1: Linear Response Theory

Last semester in 8.511, we discussed *linear response theory* in the context of charge screening and the free-fermion polarization function. This theory can be extended to a much wider range of areas, however, and is a very useful tool in solid state physics. We'll begin this semester by going back and studying linear response theory again with a more formal approach, and then returning to this like superconductivity a bit later.

1.1 Response Functions and the Interaction Representation

In solid state physics, we ordinarily think about many-body systems, with something on the order of 10^{23} particles. With so many particles, it is usually impossible to even think about a wave function for the whole system. As a result, it is often more useful for us to think in terms of the macroscopic observable behaviors of systems rather than their particular microscopic states.

One example of such a macroscopic property is the magnetic susceptibility $\chi_H \equiv \frac{\partial M}{\partial H}$, which is a measure of the response of the net magnetization M of a system to an applied magnetic field $H(\vec{r},t)$. This is the type of behavior we will be thinking about: we can mathematically probe the system with some perturbing external probe or field (*e.g.* $H(\vec{r},t)$), and try to predict what the system's response will be in terms of the expectation values of some observable quantities.

Let $\hat{H}$ be the full many-body Hamiltonian for some isolated system that we are interested in. We spent most of 8.511 thinking about how to solve for the behavior of a system governed by $\hat{H}$. As interesting as that behavior may be, we will now consider that to be a solved problem. That is, we will assume the existence of a set of eigenkets $\{|n\rangle\}$ that diagonalize $\hat{H}$ with associated eigenvalues (energies) E_n.

In addition to $\hat{H}$, we now turn on an external probe potential $\hat{V}$, such that the total Hamiltonian H_{Tot} satisfies:

$$\hat{H}_{Tot} = \hat{H} + \hat{V} \tag{1.1}$$

In particular, we are interested in probe potentials that arise from the coupling of some external scalar or vector field to some sort of "density" in the sample. For example, the external field can be an electric potential $U(\vec{r},t)$, which couples to the electronic *charge density* $\hat{\rho}(\vec{r})$ such that

$$\hat{V} = \int_V d\vec{r}\hat{\rho}(\vec{r})\, U(\vec{r},t) \tag{1.2}$$

where the electron density operator $\hat{\rho}(\vec{r})$ is given by

$$\hat{\rho}(\vec{r}) = \sum_{i=1}^{N} \delta(\vec{r} - \vec{r_i}) \tag{1.3}$$

In first quantized language, with $\vec{r}$ being the position of electron i the N-electron system. In second quantized notation, recall

$$\hat{\rho}\left(\vec{r}\right) = \Psi^{\dagger}\left(\vec{r}\right)\Psi\left(\vec{r}\right) \tag{1.4}$$

where $\Psi^{\dagger}\left(\vec{r}\right)$ and $\Psi\left(\vec{r}\right)$ are the electron field creation and annihilation operators, respectively.

The momentum space version of the electron density operator, $\hat{\rho}\left(\vec{q}\right)$, is related to $\hat{\rho}\left(\vec{r}\right)$ through the Fourier transforms:

$$\hat{\rho}\left(\vec{r}\right) = \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}\hat{\rho}\left(\vec{q}\right) \tag{1.5}$$

$$\Psi\left(\vec{r}\right) = \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}c_{\vec{k}} \tag{1.6}$$

such that

$$\hat{\rho}\left(\vec{q}\right) = \sum_{\vec{r}} e^{-i\vec{q}\cdot\vec{r}} \tag{1.7}$$

$$= \sum_{\vec{k}} c^{\dagger}_{\vec{k}-\vec{q}}c_{\vec{k}} \tag{1.8}$$

Equation (1.7) is the first quantized form of $\hat{\rho}\left(\vec{q}\right)$, and equation (1.8) is the second quantized form with $c^{\dagger}_{\vec{k}-\vec{q}}$ the creation operator for an electron with momentum[1] $\vec{k}-\vec{q}$ and $c_{\vec{k}}$ the destruction operator for an electron with momentum $\vec{k}$.

Returning to equation (1.1), we'd like to think about $\hat{V}$ as a perturbation on the external field-free system Hamiltonian $\hat{H}$. This leads us naturally to consider $\hat{H}$ as the *unperturbed* Hamiltonian within the *interaction picture* representation. Recall that this $\hat{H}$ is a very complicated beast with all of the electron-electron repulsions included, but for our purposes we just take as a given that there are a set of eigenstates and energies that diagonalize this Hamiltonian.

Recall the formulation of the interaction representation:

$$i\hbar\frac{\partial}{\partial t}|\phi\left(t\right)\rangle = \left(\hat{H}+\hat{V}\right)|\phi\left(t\right)\rangle \tag{1.9}$$

We can "unwind" the natural time dependence due to $\hat{H}$ from the state ket $|\phi\left(t\right)\rangle$ to form an interaction representation state ket $|\tilde{\phi}\left(t\right)\rangle_I$ by

$$|\tilde{\phi}\left(t\right)\rangle_I = e^{i\hat{H}t}|\phi\left(t\right)\rangle \tag{1.10}$$

$$|\phi\left(t\right)\rangle_I = e^{-i\hat{H}t}|\tilde{\phi}\left(t\right)\rangle \tag{1.11}$$

Note that in the absence of $\hat{V}$, these interaction picture state kets are actually the *Heisenberg picture* state kets of the system. Also, we have now officially set $\hbar = 1$. After substituting (1.11) into (1.9), we obtain

$$i\hbar\frac{\partial}{\partial t} = e^{i\hat{H}t}\hat{V}e^{-i\hat{H}t}|\tilde{\phi}\left(t\right)\rangle \tag{1.12}$$

$$= \hat{V}_I|\tilde{\phi}\left(t\right)\rangle \tag{1.13}$$

[1] $\vec{k}$ and $\vec{q}$ are actually wavevectors, which differ from momenta by a factor of $\hbar$. When in doubt, assume $\hbar = 1$.

where we have set

$$\hat{V}_I = e^{i\hat{H}t}\hat{V}e^{-i\hat{H}t} \tag{1.14}$$

Thus the interaction picture state ket evolves simply according to the dynamics governed solely by the interaction picture perturbing potential $\hat{V}_I$.

More generally, we can write *any* observable (operator) in the interaction picture as

$$\hat{A}_I = e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t} \tag{1.15}$$

We can integrate equation (1.12) with respect to t to get

$$|\tilde{\phi}(t)\rangle = |\phi_0\rangle - i\int_{-\infty}^{t} dt'\ \hat{V}_I(t')\,|\tilde{\phi}(t')\rangle \tag{1.16}$$

At first it seems like we have not done much to benefit ourselves, since all we have done is to convert the ordinary Schrodinger equation, a PDE, into an integral equation. However, if $\hat{V}_I$ is small, then we can iterate equation (1.16):

$$|\tilde{\phi}(t)\rangle \approx |\phi_0\rangle - i\int_{-\infty}^{t} dt'\ \hat{V}_I(t')\,|\phi_0\rangle + \cdots \tag{1.17}$$

The essence of linear response theory is that we focus ourselves on cases where $\hat{V}_I$ is sufficiently weak that the perturbation series represented by equation (1.17) has essentially converged after including just the first non-trivial term listed above. This term is *linear* in $\hat{V}_I$.

Throughout this discussion, we will be working at $T = 0$, so $|\phi_0\rangle$ is simply the ground state of the non-perturbed total system Hamiltonian $\hat{H}$. Note that we have taken our initial time, i.e. the lower limit of integration in equation (1.16), to be $-\infty$. This is because we want to imagine turning on the probing potential $\hat{V}$ *adiabatically*, that is so slowly that the system tracks the ground state for all finite times. If we were to turn on the probe sharply, the system would exhibit complicated ringing behavior that we are not interested in.

We now return to our model experiment for studying the properties of our system. After applying some probe via the external potential $\hat{V}$, we want to measure the response of some observable of the system $\hat{A}$. We characterize this response through the expectation value of $\hat{A}$, $\langle\hat{A}\rangle$:

$$\langle\hat{A}\rangle = \langle\phi(t)\,|\hat{A}\,|\phi(t)\rangle \tag{1.18}$$

$$= \langle\tilde{\phi}(t)\,|\hat{A}_I|\tilde{\phi}(t)\rangle \tag{1.19}$$

The key now is to substitute in the approximation for $|\tilde{\phi}(t)$ given by equation (1.17) into equation (1.19). Since we have only kept terms up to linear order in $\hat{V}_I$, we must be careful only to keep terms to this order. After performing this substitution, we arrive at

$$\langle\hat{A}\rangle \approx \langle\phi_0|\hat{A}|\phi_0\rangle - i\int_{-\infty}^{t} dt' e^{\eta t'}\langle\phi_0|[\hat{A}_I(\vec{r},t)\,,\hat{V}_I(t')]|\phi_0\rangle \tag{1.20}$$

The mysterious factor $e^{\eta t'}$ comes from our "adiabatic switching-on" of the potential. This ensures that the system evolves smoothly from $t = -\infty$ to t. Eventually, we will send $\eta \to 0$. Since we are interested in positive times t close to 0 when compared with $-\infty$, we don't need to worry about the $e^{\eta t'}$ messing anything up.

The other mysterious piece of equation (1.20) is the appearance of the commutator $[\hat{A}_I(\vec{r},t), \hat{V}_I(t')]$. These two terms simply come from the two possible terms linear in $\hat{V}_I$ arising from the substitutions

$$|\tilde{\phi}(t)\rangle \approx |\phi_0\rangle - i\int_{-\infty}^{t} dt' \hat{V}_I(t')\,|\phi_0\rangle$$

and

$$\langle\tilde{\phi}(t)\,| \approx \langle\phi_0| + i\int_{-\infty}^{t} dt' \hat{V}_I(t')\,\langle\phi_0|$$

Note that the integration is with respect to t', since it comes from the expression for $|\tilde{\phi}(t)\rangle$ which involves an integration of $\hat{V}_I$ with respect to t'. The observable $\hat{A}$ is also a function of space and time, but there is no reason to integrate over it at this point. This is one way to remember what to integrate over if you forget some day.

1.2 Response Functions

What we're really interested in, however, is not $\langle\hat{A}\rangle$ itself, but the change in $\langle\hat{A}\rangle$ relative to the unperturbed state:

$$\langle\delta\hat{A}\rangle = \langle\delta\hat{A}(\vec{r},t)\rangle - \langle\phi_0|\delta\hat{A}|\phi_0\rangle \tag{1.21}$$

$$= \lim_{\eta\to 0} -ie^{\eta t}\int_{-\infty}^{t} dt' e^{\eta(t'-t)}\langle\phi_0|[\hat{A}_I(\vec{r},t), \hat{V}_I(t')]|\phi_0\rangle \tag{1.22}$$

Now is when we will specialize to the specific type of probe potential describe in the previous example. For concreteness, we consider the potential of equation (1.2):

$$\hat{V} = \int_V d\vec{r}\hat{\rho}(\vec{r})\,U(\vec{r},t)$$

$U(\vec{r},t)$ commutes with the Hamiltonian, so the interaction picture representation of $\hat{V}$ is given by

$$\hat{V}_I = e^{i\hat{H}t}\int_V d\vec{r'}\ \hat{\rho}\left(\vec{r'}\right) U\left(\vec{r'},t\right) e^{-i\hat{H}t} \tag{1.23}$$

$$= \int_V d\vec{r'}\ e^{i\hat{H}t}\hat{\rho}(\vec{r'})e^{-i\hat{H}t}U\left(\vec{r'},t\right) \tag{1.24}$$

$$= \int_V d\vec{r'}\ \hat{\rho}_I(\vec{r'})\ U\left(\vec{r'},t\right) \tag{1.25}$$

Substituting this expression for $\hat{V}_I$ back into equation (1.22), we obtain:

$$\langle\delta\hat{A}(\vec{r},t)\rangle = \lim_{\eta\to 0} -ie^{\eta t}\int_{-\infty}^{t} dt' \int_V d\vec{r}\ e^{\eta(t'-t)}\ \langle\phi_0|[\hat{A}_I(\vec{r},t), \hat{\rho}_I(\vec{r}',t')]|\phi_0\rangle\ U(\vec{r}',t') \tag{1.26}$$

We define the *response function* χ as the *kernel* of this expression for $\langle\delta\hat{A}(\vec{r},t)\rangle$:

$$\langle\delta\hat{A}(\vec{r},t)\rangle = \int_{-\infty}^{\infty} dt'\ d\vec{r}'\chi(\vec{r},\vec{r}',t-t')\ U(\vec{r}',t') \tag{1.27}$$

χ is a function of $(t-t')$ only, since $\hat{H}$ is independent of time. The interpretation of equation (1.27) is that if we "shake" the system with an external potential $U(\vec{r'}, t')$, then the response of the system in terms of some observable $\hat{A}$ at the point $\vec{r}$ and time t is modulated by the response function $\chi(\vec{r}, \vec{r'}, t-t')$.

Thus from comparing this definition with equation (1.26), we see that

$$\begin{aligned}\chi(\vec{r}, \vec{r'}, t-t') \equiv & \\ & -i \, \langle\phi_0|[\hat{A}_I(\vec{r}, t), \hat{\rho}_I(\vec{r'}, t')]|\phi_0\rangle \; e^{\eta(t'-t)} \; \theta(t-t')\end{aligned} \tag{1.28}$$

Note that in equation (1.27) we extended the limits of integration from $-\infty$ to ∞ for convenience, and thus have added the Heaviside step function $\theta(t-t')$ to our definition of $\chi(\vec{r}, \vec{r'}, t-t')$. Recall that $\theta(t) = 0$ for $t < 0$ and $\theta(t) = 1$ for $t > 0$. This ensures *causality* in our definition of χ, since the system should not be able to respond to the perturbation before it happens.

Notice also that based on this definition, the response function is purely a function of the system's unperturbed Hamiltonian $\hat{H}$; U does not appear anywhere in the expression. Thus investigations of χ can reveal information about the systems Hamiltonian.

In this definition, the electron density $\hat{\rho}_I(\vec{r'}, t')$ appears because we specialized to the case of an applied external electric potential that couples to the system's charge density. For a probe that couples to some other density, such as magnetization density $\hat{m}(\vec{r'}, t')$, we can simply replace $\hat{\rho}_I(\vec{r'}, t')$ by $\hat{m}_I(\vec{r'}, t')$ in definition (1.28).

1.3 Electron Density Response to an Applied Electric Potential

In this section, we will specialize further to the case where we observe the response of the electron density to an applied potential that couples to the density. Thus we are picking $\hat{A} = \hat{\rho}$.

We begin by taking the Fourier transform of equation (1.28) with respect to time:

$$\begin{aligned}t'' &= t' - t \\ \chi(\vec{r}, \vec{r'}, \omega) &= -i \int_{-\infty}^{0} dt'' \; e^{-(i\omega-\eta)t''} \; \langle\phi_0|[\hat{\rho}_I(\vec{r}, 0), \hat{\rho}_I(\vec{r'}, t'')]|\phi_0\rangle\end{aligned} \tag{1.29}$$

Recall that we have a complete set of eigenstates of $\hat{H}$:

$$\begin{aligned}\hat{H}|n\rangle &= E_n|n\rangle \\ \sum_n |n\rangle\langle n| &= \hat{1}\end{aligned}$$

Inserting this complete set of states into the commutator

$$[\hat{\rho}_I(\vec{r}, 0), \hat{\rho}_I(\vec{r'}, t'')] = [\hat{\rho}_I(\vec{r}, 0), \sum_n |n\rangle\langle n|\hat{\rho}_I(\vec{r'}, t'')] \tag{1.30}$$

and noting that

$$\hat{\rho}_I = e^{i\hat{H}t}\hat{\rho}e^{-i\hat{H}t} \tag{1.31}$$

and

$$e^{-i\hat{H}t}|n\rangle = e^{-iE_n t}|n\rangle \tag{1.32}$$

we obtain

$$\chi(\vec{r},\vec{r}',\omega) = -i \int_{-\infty}^{0} dt'' \sum_n \langle\phi_0|\hat{\rho}(\vec{r})|n\rangle\langle n|\hat{\rho}(\vec{r}')|\phi_0\rangle \; e^{i(E_n-E_0)t''-(i\omega-\eta)t''} \tag{1.33}$$

$$- \sum_n \langle\phi_0|\hat{\rho}(\vec{r}')|n\rangle\langle n|\hat{\rho}(\vec{r})|\phi_0\rangle \; e^{-i(E_n-E_0)t''-(i\omega-\eta)t''} \tag{1.34}$$

All of the time dependence has now been brought up into the exponentials, so it is trivial to perform the integration over time. This yield the *spectral representation* of $\chi(\vec{r},\vec{r}',\omega)$:

$$\chi(\vec{r},\vec{r}',\omega) = \sum_n \left[\frac{\langle\phi_0|\hat{\rho}(\vec{r})|n\rangle\langle n|\hat{\rho}(\vec{r}')|\phi_0\rangle}{\omega-(E_n-E_0)+i\eta} - \frac{\langle\phi_0|\hat{\rho}(\vec{r}')|n\rangle\langle n|\hat{\rho}(\vec{r})|\phi_0\rangle}{\omega+(E_n-E_0)+i\eta} \right] \tag{1.35}$$

If there is *translational invariance* in the sample, then the response function $\chi(\vec{r},\vec{r}',\omega)$ should be simply a function of the difference $\vec{r}-\vec{r}'$. In this case, the spatial Fourier transform is simple:

$$\chi(\vec{q},\omega) = \frac{1}{V}\int d\vec{r}\; d\vec{r}' \; e^{-i\vec{q}\cdot(\vec{r}-\vec{r}')} \; \chi(\vec{r}-\vec{r}',\omega) \tag{1.36}$$

$$= \sum_n \left[\frac{\langle\phi_0|\hat{\rho}(\vec{q})|n\rangle\langle n|\hat{\rho}(-\vec{q})|\phi_0\rangle}{\omega-(E_n-E_0)+i\eta} - \frac{\langle\phi_0|\hat{\rho}(-\vec{q})|n\rangle\langle n|\hat{\rho}(\vec{q})|\phi_0\rangle}{\omega+(E_n-E_0)+i\eta} \right] \tag{1.37}$$

where $\hat{\rho}(\vec{q}) \equiv \hat{\rho}_{\vec{q}}$ is given by equations (1.7) and (1.8) in first quantized or second quantized notation, respectively.

Since the electron density $\hat{\rho}(\vec{r})$ is a *real* function, we have the important relation

$$\hat{\rho}_{-\vec{q}} = \hat{\rho}_{\vec{q}}^{\dagger} \tag{1.38}$$

which is a simple consequence of the nature of the Fourier transform. This implies that

$$\langle\phi_0|\hat{\rho}(\vec{q})|n\rangle\langle n|\hat{\rho}(-\vec{q})|\phi_0\rangle = |\langle n|\hat{\rho}^{\dagger}(\vec{q})|\phi_0\rangle|^2 \tag{1.39}$$

Using this along with the relation

$$\mathrm{Im}\left\{\frac{1}{x+i\eta}\right\} = -\pi\delta(x) \tag{1.40}$$

we arrive at the next important result:

$$\mathrm{Im}\{\chi(\vec{q},\omega)\} = -\pi\sum_n \{|\langle n|\hat{\rho}^{\dagger}(\vec{q})|\phi_0\rangle|^2\delta\left(\omega-(E_n-E_0)\right) \tag{1.41}$$

$$-|\langle n|\hat{\rho}(\vec{q})|\phi_0\rangle|^2\delta\left(\omega+(E_n-E_0)\right)\} \tag{1.42}$$

Why are we interested in the imaginary part of χ? The imaginary part of χ gives us information about *dissipation*, i.e. the absorption and loss of energy as a result of the interaction with the probe. We will often use the notation

$$\chi''(\vec{q},\omega) = \mathrm{Im}\{\chi(\vec{q},\omega)\}$$

We can plot $\chi''(\vec{q},\omega)$ as a function of ω for fixed $\vec{q}$ (see plot). The location of the peaks tells us about the types of excitations being produced. As we will see shortly, it actually turns out that knowledge of $\chi''(\vec{q},\omega)$ is all we need; the real part of $\chi(\vec{q},\omega)$, denoted $\chi'(\vec{q},\omega)$, can be reconstructed from $\chi''(\vec{q},\omega)$ alone.

1.4 Sanity Check: Free Fermions

To convince ourselves that of this formalism is really working, we will try it out on the case of free fermions, which we studied last semester in 8.511. Now, $\chi(\vec{q},\omega)$ is simply $\Pi_0(\vec{q},\omega)$. The ground state for free fermions is just the simple spherical Fermi sea, filled up to exactly to the Fermi energy. The excited states are of the form

$$|n_{\vec{k}}\rangle = |\text{hole at } \vec{k},\ e^- \text{ at } \vec{k}+\vec{q}\rangle \tag{1.43}$$

These single particle-hole excitations are the only types of excitations possible in this case, since the external field U couples to the density $\hat{\rho}_{\vec{q}} = \sum_{\vec{k}} c^\dagger_{\vec{k}-\vec{q}} c_{\vec{k}}$. The matrix elements we need are simple to calculate as well, since all that is required is a filled initial state below the Fermi sea (with wave vector $\vec{k}$ and an open state above the Fermi sea with wave vector $\vec{k}+\vec{q}$ to jump into. Thus

$$\langle n_{\vec{k}}|\hat{\rho}^\dagger_{\vec{q}}|\phi_0\rangle = (1-f_{\vec{k}+\vec{q}})f_{\vec{k}} \tag{1.44}$$

where $f_{\vec{k}}$ is 1 if the state with momentum $\vec{k}$ is occupied in the ground state, and 0 if it is empty.

Substituting this in, we get

$$\Pi_0(\vec{q},\omega) = \sum_{\vec{k}} \left[\frac{(1-f_{\vec{k}+\vec{q}})f_{\vec{k}}}{\omega - (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}) + i\eta} - \frac{(1-f_{\vec{k}-\vec{q}})f_{\vec{k}}}{\omega + (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}) + i\eta} \right] \tag{1.45}$$

Letting

$$\vec{k} - \vec{q} = \vec{k}'$$
$$\vec{k} = \vec{k}' + \vec{q}$$

we can switch the dummy summation variables on the second term and combine both terms into one:

$$\Pi_0(\vec{q},\omega) = \sum_{\vec{k}} \frac{(1-f_{\vec{k}+\vec{q}})f_{\vec{k}} - (1-f_{\vec{k}})f_{\vec{k}+\vec{q}}}{\omega - (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}) + i\eta} \tag{1.46}$$

$$= \sum_{\vec{k}} \frac{f_{\vec{k}} - f_{\vec{k}+\vec{q}}}{\omega - (\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}}) + i\eta} \tag{1.47}$$

$$\tag{1.48}$$

This is exactly the Lindhardt formula that we derived in 8.511.

1.5 The Correlation Function $S(\vec{r},t)$

Let's switch gears now and talk about another object that we will see is related to the response function. We define the *correlation function*

$$S(\vec{r},t) = \langle\phi_0|\ \hat{\rho}_H(\vec{r},t)\hat{\rho}_H(0,0)\ |\phi_0\rangle \tag{1.49}$$

$S(\vec{r},t)$ described *fluctuations* of the electron density across the sample in space and time. Due to the translational invariance of the sample, we arbitrarily set one of arguments to $(\vec{r'},t') = (0,0)$

and observe the density correlation with another point $(\vec{r},t)$. What we want to show next is that there is a relationship between *dissipation* and *fluctuations*.

Fourier transforming $S(\vec{r},t)$ in space yields

$$S(\vec{q},t) = \langle\phi_0|\ \hat{\rho}_H(\vec{q},t)\hat{\rho}_H(-\vec{q},0)\ |\phi_0\rangle \tag{1.50}$$

$$= \sum_n |\langle n|\hat{\rho}^\dagger_{\vec{q}}|\phi_0\rangle|^2 e^{-i(E_n-E_0)t} \tag{1.51}$$

where the second line follows by inserting a complete set of states between the density operators and acting the $e^{\pm i\hat{H}t}$ operators on the eigenstates to the left and the right. Notice that this is very similar with what we did earlier on our way to deriving the form of the response function.

Now we take the Fourier transform in time:

$$S(\vec{q},\omega) = \int d\vec{r} \int dt\ e^{i\omega t} e^{-i\vec{q}\cdot\vec{r}} S(\vec{q},t) \tag{1.52}$$

$$= 2\pi \sum_n |\langle n|\hat{\rho}^\dagger_{\vec{q}}|\phi_0\rangle|^2 \delta\left(\omega - (E_n - E_0)\right) \tag{1.53}$$

This expression for $S(\vec{q},\omega)$ is identical to the first (absorptive) term in the expression for the imaginary part of the response function $\chi''(\vec{q},\omega)$. This can be restated as the Zero-Temperature Fluctuation-Dissipation Theorem:

$$\chi''(\vec{q},\omega) = -\frac{1}{2}\left(S(\vec{q},\omega) - S(-\vec{q},-\omega)\right) \tag{1.54}$$

This shows that the energy absorbed in a probing experiment of the type described in this lecture is directly related to density fluctuations across the system. Although so far we have derived everything at $T = 0$, the Fluctuation-Dissipation Theorem can be extended to finite temperatures as well. Using the thermal average

$$\langle\hat{A}\rangle_T = \frac{\mathrm{Tr}\left(e^{-\beta\hat{H}}\hat{A}\right)}{\mathrm{Tr}\left(e^{-\beta\hat{H}}\right)} \tag{1.55}$$

the derivation can be redone to arrive at the finite temperature Fluctuation-Dissipation Theorem:

$$\chi''(\vec{q},\omega) = \frac{1}{2}\left(e^{-\beta\omega} - 1\right) S(\vec{q},\omega) \tag{1.56}$$

$$S(\vec{q},\omega) = -2\left(n_B(\omega) + 1\right)\chi''(\vec{q},\omega) \tag{1.57}$$

where $n_B(\omega)$ is the Boltzmann statistical factor

$$n_B(\omega) = \frac{1}{e^{\beta\omega} - 1} \tag{1.58}$$

By playing with these relations, we can further derive the following two results:

$$S(-\vec{q},-\omega) = e^{-\beta\omega} S(\vec{q},\omega) \tag{1.59}$$

$$\chi''(\vec{q},\omega) = -\chi''(-\vec{q},-\omega) \tag{1.60}$$

Equation (1.59) is simply a statement of the law of *detailed balance*.

1.6 Measuring $S(\vec{q},\omega)$

It is possible to measure $S(\vec{q},\omega)$ directly through scattering experiments. Depending on the particle density of interest, the scattering can be performed using electrons, X-rays, neutrons, etc. This process is governed by the interaction Hamiltonian

$$\hat{H}_{int} = \sum_i v(\vec{r}_i - \vec{R}) \tag{1.61}$$

$$= \sum_{\vec{q}} e^{i(\vec{r}_i - \vec{R})\cdot q} v_{\vec{q}} \tag{1.62}$$

$$= \sum_{\vec{q}} v_{\vec{q}}\, \hat{\rho}^\dagger_{\vec{q}}\, e^{-i\vec{q}\cdot\vec{R}} \tag{1.63}$$

where $\vec{R}$ is the position of the scattering electron and $\{\vec{r}_i\}$ are the sample electrons' coordinates.

For now, we imagine probing the electron density by sending in high energy (10 - 100 keV) electrons. These electrons interact with the electrons in the sample through the Coulomb interaction. Thus

$$v_{\vec{q}} = \frac{4\pi e^2}{q^2} \tag{1.64}$$

If we wanted to perform neutron scattering, then the $\{\vec{r}_i\}$ would be the sample's *nuclear* coordinates, and the interaction would be the contact potential

$$v_{\vec{r}} = \frac{2\pi b}{M_n}\delta(\vec{r}) \tag{1.65}$$

To ensure single-scattering, we need to work in the regime of *weak coupling*. Thus we can apply the first order Born Approximation and Fermi's Golden Rule to obtain the scattering rate

$$W_{i\to f} = \frac{2\pi}{\hbar}|\langle f|\hat{H}_{int}|i\rangle|^2\delta(E_i - E_f) \tag{1.66}$$

We take the initial and final states of our scattering probe to be plane waves $|\vec{k}_i\rangle$ and $|\vec{k}_f\rangle$, respectively. Then the initial and final states of the system are

$$|i\rangle = |\phi_0\rangle \otimes |\vec{k}_i\rangle \tag{1.67}$$

$$|f\rangle = |n\rangle \otimes |\vec{k}_f\rangle \tag{1.68}$$

Let

$$\vec{Q} = \vec{k}_i - \vec{k}_f$$
$$\omega = E_{\vec{k}_i} - E_{\vec{k}_f}$$

so that $\omega > 0$ when energy is *lost* to the system and $\vec{Q}$ is the momentum transfer *to the system*. Then[2]

$$W_{i\to f} = 2\pi \sum_n \left| \sum_{\vec{q}} v_{\vec{q}}\, \langle n|\hat{\rho}^\dagger_{\vec{q}}|\phi_0\rangle \int d\vec{R}\; e^{i(\vec{k}_f - \vec{k}_i)\cdot\vec{R}} e^{-i\vec{q}\cdot\vec{R}} \right|^2 \delta\left(\omega - (E_n - E_0)\right) \tag{1.69}$$

[2] $\hbar = 0$ again.

$$= |v_{\vec{Q}}|^2 \; 2\pi \sum_n |\langle n|\hat{\rho}^\dagger_{\vec{Q}}|\phi_0\rangle|^2 \; \delta(E_f - E_i) \tag{1.70}$$

$$= |v_{\vec{Q}}|^2 \; S(\vec{Q},\omega) \tag{1.71}$$

Thus the scattering rate for scattering with a momentum transfer $\vec{Q}$ and energy loss $\hbar\omega$ is related to the correlation function $S(\vec{Q},\omega)$ very simply through a scaling by the square of the $\vec{Q}^{th}$ Fourier component of the interaction potential.