May 13

Fluctuations

Several times in the course, we have encountered formulae that relate the response of a thermodynamic system to a perturbation to an equilibrium expectation value that computes a mean-square fluctuation. For example,

$$C_V = \frac{\partial E}{\partial T} = \frac{1}{T^2}\left[\langle \mathcal{H}^2\rangle - \langle \mathcal{H}\rangle^2\right]$$

$$\chi = \frac{\partial M}{\partial h} = \frac{1}{T}\left[\langle M^2\rangle - \langle M\rangle^2\right]$$

We have also studied local correlation functions at fixed time, such as

$$\langle M(x)\, M(0)\rangle$$

to understand the concepts of correlation length and long-range order. There is more to say about the formalism of correlation functions, and now I will break briefly from our discussion of phases and critical points to discuss this theory.

In this lecture, I will use the following notation: Let $S(\vec{x})$ be the local density that integrates to the order parameter, for example,

$$\mathcal{M} = \int d^3x\; S(x)$$

and let $f(\vec{x})$ be the local field that couples to $S(\vec{x})$

$$\delta\mathcal{H} = -\int d^3x\; S(x) f(x)$$

For example, $S(\vec{x})$ might be the magnetization density and $f(\vec{x})$ the local field that couples to this local magnetization. Or, $S(\vec{x})$ could be the local extension of a rubber band, and $f(\vec{x})$ the force applied at the point $\vec{x}$. I will assume that we are in the unordered phase $T > T_C$, so that

$$\langle S(x) \rangle = 0$$

in equilibrium. If $T < T_C$, so that $\langle S(\vec{x}) \rangle = S_0 \neq 0$, most of the results I will discuss apply to the fluctuation $(S(\vec{x}) - S_0)$.

Consider first the situation with a uniform f. We have

$$\langle S(x) \rangle = \frac{\sum_{s_i} e^{-\beta H + \beta \int d^3y \, S(y) f(y)}}{\sum_{s_i} e^{-\beta H + \beta \int d^3y \, S(y) f(y)}} S(x)$$

To leading order in f,

$$\frac{\partial \langle S(x) \rangle}{\partial f} = \beta \cdot \langle S(\vec{x}) \int d^3y \, S(\vec{y}) \rangle$$

It is easy to generalize this formula to an $f(\vec{x})$ that varies over space. In that case,

$$\langle S(x) \rangle = \beta \langle S(\vec{x}) \int d^3y \, S(\vec{y}) f(\vec{y}) \rangle$$

or

$$\langle S(x) \rangle_f = \int d^3y \; \beta \langle S(x) S(y) \rangle \; f(y)$$

A formula of this type, which expresses relation, through a nonlocal kernal, between the applied field $f(\vec{x})$ and the response $\langle S(\vec{x}) \rangle$, is called a *linear response formula.*

To go further, I will make a several basic assumptions about the system that we are dealing with. I will assume that this system is translation-invariant, reflection-invariant, and time-reversal invariant. This will lead to a number of simplifications. More complicated formulae of the same general flavor will hold when these assumptions are not valid. For example, a material in an external magnetic field is not time-reversal invariant, so if $\left\langle S(\vec{x}) S(\vec{0}) \right\rangle$ must be evaluated in a nonzero field, an appropriately corrected formalism must be used.

I will now introduce Fourier representations for $f(\vec{x})$ and for $\left\langle S(\vec{x}) S(\vec{0}) \right\rangle$, using the assumptions of the previous paragraph to simplify these expressions. By translation invariance,

$$\langle S(\vec{x}) S(\vec{y}) \rangle = \langle S(\vec{x}-\vec{y}) S(\vec{0}) \rangle$$

Then we can write

$$C(\vec{x}-\vec{y}) = \langle S(\vec{x}) S(\vec{y}) \rangle$$

and express $C(\vec{x})$ and $f(\vec{x})$ in Fourier space,

$$C(\vec{x}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} \, C(\vec{k}) \qquad f(\vec{x}) = \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} \, f(\vec{k})$$

Put these expressions into the linear response formula above. We find

$$\begin{aligned}
\langle S(\vec{x}) \rangle_f &= \int \frac{d^3k}{(2\pi)^3} e^{i\vec{k}\cdot\vec{x}} \langle S_k \rangle_f \\
&= \int d^3y \;\; \beta \int \frac{d^3k \, d^3k'}{(2\pi)^3 (2\pi)^3} e^{i\vec{k}\cdot(\vec{x}-\vec{y})} e^{i\vec{k}'\cdot\vec{y}} \, C(\vec{k}) \, f(\vec{k}') \\
&= \beta \int \frac{d^3k \, d^3k'}{(2\pi)^6} e^{i\vec{k}\cdot\vec{x}} \, C(\vec{k}) \, f(\vec{k}') \, (2\pi)^3 \delta(\vec{k}-\vec{k}')
\end{aligned}$$

Thus,

$$\langle S_k \rangle_f = \frac{1}{T} C(\vec{k}) f(\vec{k})$$

We can then write the general linear response form of the relation between $\langle S(\vec{x})\rangle$ and $f(\vec{x})$ as

$$\langle S(\vec{x})\rangle = \int d^3y \, \chi(\vec{x-y}) f(\vec{y}) \quad \text{or} \quad \langle S_k \rangle = \chi(\vec{k}) f(\vec{k})$$

where the *static response function* $\chi(\vec{x} - \vec{y})$ is given by

$$\chi(\vec{x-y}) = \frac{1}{T} C(\vec{x-y})$$

The generalization of this discussion to a time-dependent response function is more subtle. The general linear response to a time-dependent field $f(\vec{x}, t)$ would be written

$$\langle S(\vec{x},t)\rangle = \int d^3x' \, dt' \quad \chi(\vec{x-x'}, t-t') \, f(\vec{x}', t')$$

The time-dependent response function must respect causality: The response must come *after* the perturbation is applied. Then

$$\chi(\vec{x},t) = 0 \quad \text{for} \quad t<0$$

This constraint has a specific implication in Fourier space that I discuss in a moment. First, though, I must develop the formalism a bit further.

To begin, write the Fourier transform of a function of space and time as

$$f(\vec{x},t) = \int \frac{d\omega}{2\pi} \frac{d^3k}{(2\pi)^3} \, e^{-i\omega t + i\vec{k}\cdot\vec{x}} \, f(\vec{k},\omega)$$

The linear response relation is a convolution, so its Fourier transform is

$$\langle S(\vec{k},\omega)\rangle = \chi(\vec{k},\omega) \, f(\vec{k},\omega)$$

The symmetries of the problem put restrictions on the reality properties of $\chi(\vec{k},\omega)$. First, since,

$$\chi(k,\omega) = \int dt \, d^3x \, e^{i\omega t} e^{-i\vec{k}\cdot\vec{x}} \, \chi(\vec{x},t)$$

if $\chi(\vec{x},t)$ is real-valued, then

$$\chi(-\vec{k},-\omega) = [\chi(k,\omega)]^*$$

If the system is symmetric under inversion

$$\chi(\vec{x},t) = \chi(-\vec{x},t) \qquad \text{or} \qquad \chi(\vec{k},\omega) = \chi(-\vec{k},\omega)$$

so

$$\chi(\vec{k},\omega) = [\chi(\vec{k},-\omega)]^*$$

Write χ as a sum of real and imaginary parts

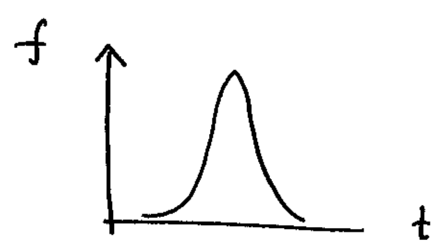
$$\chi(\vec{k},\omega) = \chi'(\vec{k},\omega) + i\,\chi''(\vec{k},\omega)$$

Then these components have the symmetry

$$\chi'(\vec{k},-\omega) = +\chi'(\vec{k},\omega) \qquad \chi''(\vec{k},-\omega) = -\chi''(\vec{k},\omega)$$

The real and imaginary parts of χ have different physical significance. The real part of χ is the direct, in-phase, response of S to f. If f is an electromagnetic wave and S is a polarization, $\chi' = \mathrm{Re}\,\chi$ is the part of the response that adds coherently with the wave and contributes to the index of refraction. On the other hand, for $\chi'' = \mathrm{Im}\,\chi$, the i indicates a response that is 90° out of phase with the driving signal This may be seen to be a response that dissipates energy from the time-dependent field f into the medium. In the case of an electromagnetic wave, χ'' contributes to the absorption.

To make this explicit, compute the work done on the system by a pulse of $f(\vec{x},t)$



The work done in an interval Δt is

$$\Delta W = \int d^3x \; f(\vec{x},t)\; \Delta S(\vec{x},t)$$

Then the total work on in a pulse is

$$W = \int dt\, d^3x \; f(x,t) \; \frac{\partial}{\partial t} S(x,t)$$

Insert the Fourier representation of $f(\vec{x},t)$ and $S(\vec{x},t)$. Since

$$f(\vec{x},t) = \int \frac{d\omega\, d^3k}{(2\pi)^4} \; e^{-i\omega t} e^{+i\vec{k}\cdot\vec{x}} \; f(\vec{k},\omega)$$

if $f(\vec{x},t)$ is real,

$$f(-\vec{k},-\omega) = [f(\vec{k},\omega)]^*$$

Then

$$W = \int dt\, d^3x \int \frac{d\omega'\, d^3k'}{(2\pi)^4} \; e^{-i\omega' t} e^{i\vec{k}'\cdot\vec{x}} \int \frac{d\omega\, d^3k}{(2\pi)^4} \; e^{-i\omega t} e^{i\vec{k}\cdot\vec{x}}$$

$$\cdot\, f(\vec{k}',\omega') \cdot (-i\omega) \; S(\vec{k},\omega)$$

$$= \int \frac{d\omega\, d^3k}{(2\pi)^4} -i\omega f(-\vec{k},-\omega) \; S(\vec{k},\omega) = \int \frac{d\omega\, d^3k}{(2\pi)^4} -i\omega f(-k,-\omega) \chi(k,\omega) \, f(k,\omega)$$

so that finally

$$W = \int \frac{d\omega\, d^3k}{(2\pi)^4} \;\; [-i\omega\, \chi(\vec{k},\omega)] \;\; |f(k,\omega)|^2$$

The real part of $\chi(\vec{k},\omega)$ is even under $\omega \rightarrow -\omega$. Then the quantity $\omega\, \mathrm{Re}\, \chi(\vec{k},\omega)$ is *odd* and integrates to zero. What remains is

$$W = \int \frac{d\omega\, d^3k}{(2\pi)^4} \quad \omega \chi''(\vec{k},\omega) \quad \cdot \left| f(\vec{k},\omega) \right|^2$$

Thus, the dissipation of energy in the medium is a convolution of the *imaginary part* of χ with the square of f.

For a stable system in equilibrium, any time-dependent force should deposit, not extract, energy. This implies that

$$\omega \chi''(\vec{k},\omega) > 0$$

A wayt to think about the form of $\chi(\vec{x},t)$ is that it is built up from responses that can be excited suddenly, decay exponentially, and also can *ring* at some frequency. Contributions to χ with this description are the sum of terms

$$A\, e^{-i\alpha t} e^{-\gamma t} \cdot \Theta(t)$$

The Fourier transform of this structure is

$$\int_{-\infty}^{\infty} dt \quad e^{i\omega t} \left\{ A\, e^{-i\alpha t} e^{-\gamma t} \Theta(t) \right\}$$

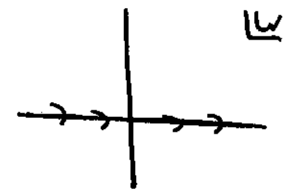
$$= \int_0^{\infty} dt \quad A \quad e^{i\omega t - i\alpha t - \gamma t} \qquad = \qquad \frac{A}{\gamma + i\alpha - i\omega}$$

$$= \qquad \frac{iA}{\omega - (\alpha - i\gamma)}$$

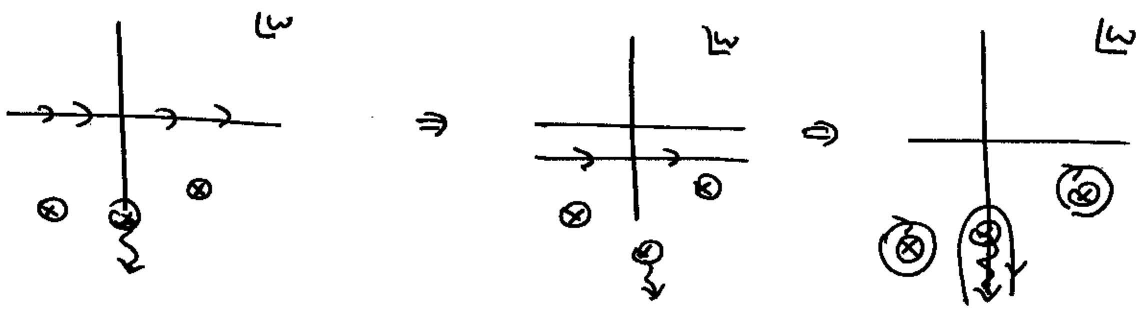
As an analytic function of ω, this is a function with one pole, in the lower half ω plane.

The location of the analytic singularities of $\chi(\vec{k},\omega)$ in the lower half plane is a general requirement that implements the constraint of causality. To see this, consider inverting the Fourier transform

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



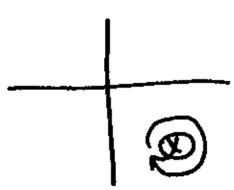
The integral is over *real* ω; it runs along the real axis of the complex ω plane. I will assume that $\chi(k,\omega)$ falls off fast enough as $|\omega| \to \infty$ that we can ignore contributions to the integral at large real values of ω. Then we can evaluate the integral by contour deformation. For $t > 0$, we push the contour downward and pick up contributions from any singularities the we encounter,



A singularity at $\omega = \alpha - i\gamma$ leads to a contribution that behaves in real time as

$$e^{-i\alpha t}\, e^{-\gamma t}$$

For the function given above, we can explicitly compute the contribution from the pole at $\omega = \alpha - i\gamma$. We find



$$= -2\pi i \,\mathrm{Res}\left\{ \frac{1}{2\pi} \frac{iA\, e^{-i\omega t}}{\omega - (\alpha - i\gamma)} \right\}$$

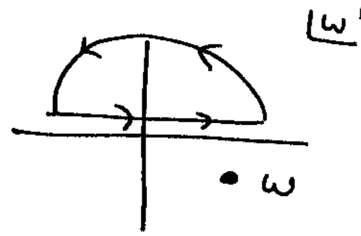
$$= A\, e^{-i\alpha t}\, e^{-\gamma t}$$

as expected.

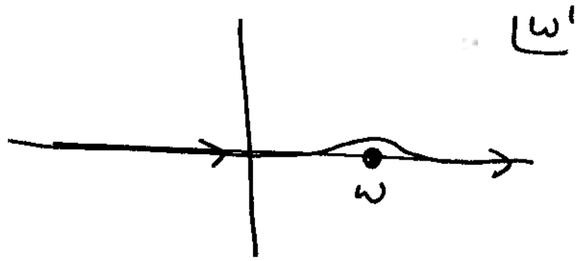
For $t < 0$, the exponential $e^{-i\omega t}$ *increases* as the contour is pushed downward but *decreases* as the contour is pushed upward. We then evaluate the integral in this region by pushing the contour up to $\mathrm{Im}\,\omega \to \infty$. Any singularity that we encounter in this process gives a nonzero contribution to $\chi(\vec{x}, t)$ for $t < 0$. Causality insists that there should be no such contribution. then, as a requirement of causality, $\chi(\vec{k}, \omega)$ must be *analytic in the upper half ω plane.*

As a consequence of this analytic structure, the contour integral in the ω plane must be zero

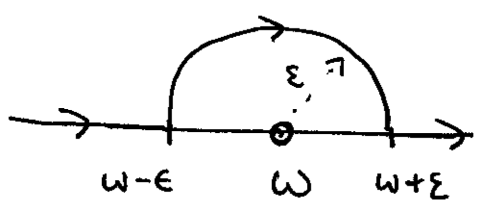
$$\oint \frac{d\omega'}{2\pi} \frac{\chi(\vec{k},\omega')}{\omega'-\omega} = 0$$



as long as the contour is a path in the upper half plane and ω is a point in the lower half plane. If we bring both the contour and ω to the real axis, the integral remains zero.



The contour must remain above the pole. To achieve this , the contour must make a small detour around the pole.



In this context, it is conventional to define the *principal value* of an integral over ω as the value of the integral excluding a symmetric interval around the pole.

$$\mathcal{P}\int_{-\infty}^{\infty} d\omega' \, \frac{f(\omega')}{\omega'-\omega} = \left(\int_{\omega+\epsilon}^{\infty} d\omega' + \int_{-\infty}^{\omega-\epsilon} d\omega' \right) \frac{f(\omega')}{\omega'-\omega}$$

This integral is finite. The principal value accounts for the full integral above except for the semicircular detour. That contribution equals $(-\frac{1}{2})$ times the residue of the pole. In all, the integral that we are discussing evaluates to

$$\oint \frac{d\omega'}{2\pi} \, \frac{\chi(\vec{k},\omega')}{\omega'-\omega} = \mathcal{P}\int \frac{d\omega'}{2\pi} \, \frac{\chi(\vec{k},\omega')}{\omega'-\omega} - \frac{i}{2}\chi(\vec{k},\omega)$$

The statement that the integral equals zero gives a relation between the real and imaginary parts of $\chi(\vec{k},\omega)$. Taking the imaginary part of the integral,

$$0 = \mathcal{P}\int \frac{d\omega'}{2\pi} \, \frac{\chi''(\vec{k},\omega')}{\omega'-\omega} - \frac{1}{2}\chi'(\vec{k},\omega)$$

Then the real part χ' can be expressed in terms of the imaginary part χ''

$$\chi'(k,\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty} d\omega' \, \chi''(k,\omega') \frac{1}{\omega'-\omega}$$

Using the antisymmetry of χ'',

$$= \frac{1}{\pi}\mathcal{P}\int_{0}^{\infty} d\omega' \, \chi''(k,\omega') \left[\frac{1}{\omega'-\omega} - \frac{1}{-\omega'-\omega} \right]$$

so that, finally,

$$\chi'(k,\omega) = \frac{2}{\pi}\mathcal{P}\int_{0}^{\infty} d\omega' \, \frac{\omega' \chi''(k,\omega')}{(\omega')^2 - \omega^2}$$

Taking the real part of the integral, we can derive a reciprocal relation

$$\chi''(k,\omega) = -\frac{2\omega}{\pi} \mathcal{P} \int_0^\infty d\omega' \frac{\chi'(k,\omega')}{(\omega')^2 - \omega^2}$$

These are called the *Kramers-Krönig relations.* They connect the direct linear response and the dissipative response to an applied perturbation.

We are now ready to discuss the computation of the time-dependent response function in terms of the time-dependent correlation function. Earlier in this lecture, I wrote the relation for the *static* response function and the *equal-time* correlation function

$$\chi(\vec{x}) = \beta \cdot \langle S(\vec{x})\, S(\vec{0}) \rangle = \beta\, C(\vec{x})$$

I will now discuss how this result generalizes to time-dependent quantities. I apologize that I will not give complete proofs of the final results. This would require a great deal of theoretical equipment. I hope that, in any event, these results will be well motivated.

If we use the formula for time-dependent response to represent the response to a static force, we find

$$\langle S(\vec{x},t) \rangle = \int dt'\, d^3x'\;\; \chi(\vec{x}-\vec{x}', t-t')\; f(\vec{x}')$$

or, after a spatial Fourier transform

$$\langle S(\vec{k},t) \rangle = \int dt' \;\; \chi(\vec{k}, t-t')\; f(\vec{k})$$

Now set $t = 0$. By causality

$$\langle S(\vec{k}, t=0)\rangle = \int_{-\infty}^{0} dt' \; \chi(\vec{k}, -t') \, f(\vec{k})$$

or

$$\langle S(\vec{k})\rangle = \left[\int_{0}^{\infty} dt \; \chi(\vec{k}, t) \right] \cdot f(\vec{k})$$

This should be compared to our earlier formula

$$\langle S(\vec{k})\rangle = \beta \, C(\vec{k}) \, f(\vec{k})$$

where $C(\vec{k})$ is the Fourier transform of the static or equal-time correlation function,

$$C(\vec{x}) = \langle S(\vec{x}) \, S(0)\rangle \qquad \underline{\text{equal}} \ \underline{\text{times}}$$

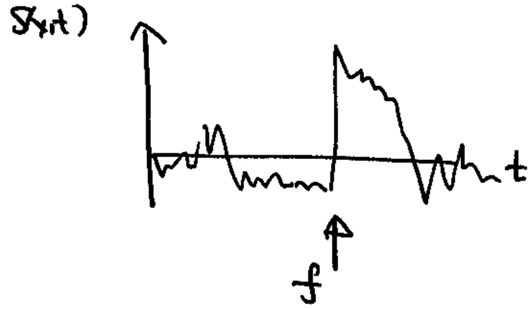
Generalize this object to the time-dependent case,

$$C(\vec{x}, t) = \langle S(\vec{x}, t) \, S(\vec{0}, 0)\rangle$$

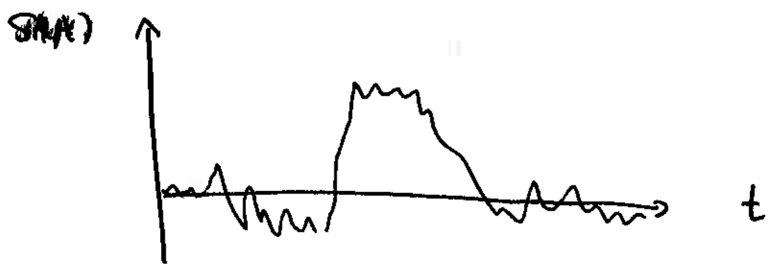
Then the formulae match if we set

$$\chi(\vec{k}, t) = -\beta \frac{\partial}{\partial t} C(\vec{k}, t) \cdot \Theta(t)$$

This is the correct answer. This formula is also motivated by the following physical argument: The response function $\chi(\vec{k}, t)$ is the response to a fluctuation of $S(\vec{k}, t)$ induced by a fluctuating force applied at the time $t = 0$,



Such a fluctuation can also appear spontaneously, as the result of a thermal fluctuation at $t = 0$ or earlier.



In these two cases, the fluctuation should decay in a similar manner and, in particular, with the same time constants.

If the system is *time-reversal invariant*, then

$$\langle S(\vec{x},t)\, S(0,0) \rangle = \langle S(\vec{x},-t)\, S(0,0) \rangle$$

In Fourier space

$$C(\vec{k},\omega) = \int \frac{d\omega}{2\pi}\, e^{i\omega t}\, C(\vec{k},t)$$

this implies

$$C(\vec{k},\omega) = C(\vec{k},-\omega)$$

Then $C(\vec{k},\omega)$ is a *real, symmetric* function. On the other hand, $\chi(\vec{k},\omega)$ is not symmetric, due to the requirement from causality that

$$\chi(\vec{k},t) = 0 \quad \text{for} \quad t<0$$

The Fourier transform of χ is predicted to be

$$\chi(\vec{k},\omega) = \int_{-\infty}^{\infty} dt \; e^{i\omega t} \; \chi(\vec{k},t)$$

$$= \int_{0}^{\infty} dt \; \left[-\beta \frac{\partial}{\partial t} C(\vec{k},t)\right] e^{i\omega t}$$

Integrating this by parts, we find

$$\chi(\vec{k},\omega) = -\beta C(\vec{k},t)\, e^{i\omega t} \Big|_0^{\infty} + i\beta\omega \int_0^{\infty} dt \; e^{i\omega t} C(\vec{k},t)$$

$$= \beta C(\vec{k},t=0) + i\beta\omega \int_0^{\infty} dt \; e^{i\omega t} C(\vec{k},t)$$

The first term in the second line is real. The the imaginary part of χ is

$$\chi''(\vec{k},\omega) = \beta\omega \int_0^{\infty} dt \; \cos\omega t \; C(\vec{k},t)$$

$$= \beta\omega \int_0^{\infty} dt \; \tfrac{1}{2}\left(e^{i\omega t} + e^{-i\omega t}\right) C(\vec{k},t)$$

Using the symmetry of $C(\vec{k},t)$,

$$\chi''(\vec{k},\omega) = \frac{\beta\omega}{2}\int_{-\infty}^{\infty} dt \; e^{i\omega t} \, C(\vec{k},t)$$

so that, finally,

$$\chi''(\vec{k},\omega) = \frac{\beta\omega}{2} \, C(\vec{k},\omega)$$

If we use this expression in the earlier formula for the work done by a pulse $f(\vec{x},t)$, we find

$$W = \int \frac{d\omega \, d^3k}{(2\pi)^4} \quad \frac{\beta\omega^2}{2} \, C(\vec{k},\omega) \quad |f(\vec{k},\omega)|^2$$

This formula is called the *fluctuation-dissipation theorem.*

These formula have a straightforward generalization to quantum systems. Again, I will motivate, rather than fully deriving, the key results. In the quantum case, $S(\vec{x},t)$ is an operator

$$S(\vec{x},t) = e^{iHt} \, S(\vec{x},0) \, e^{-iHt}$$

This operator $S(\vec{x},t)$ is the *quantum field* in the sense that I described in the previous lecture. In general, operators $S(\vec{x},t)$ do not commute at unequal times. It can be shown that the response function is proportional to the commutator

$$\chi''(\vec{x}-\vec{x}',t-t') = \frac{1}{2\hbar} \langle [S(\vec{x},t), S(\vec{x}',t')] \rangle \; \Theta(t-t')$$

where the expectation value is that of quantum statistical mechanics

$$\langle A \rangle = \frac{1}{Z} \operatorname{tr}\left[A e^{-\beta H}\right]$$

We can manipulate the right-hand side of the equation for χ'' as follows: First, using translation invariance,

$$\langle S(\vec{x},t)\, S(\vec{x}',t') \rangle = \langle S(\vec{x}-\vec{x}', t-t')\, S(0,0) \rangle$$

Similarly, the second term in the commutator can be written as

$$\langle S(\vec{x}',t')\, S(\vec{x},t) \rangle = \langle S(0,0)\, S(\vec{x}-\vec{x}', t-t') \rangle$$

The numerator of this expression is

$$\operatorname{tr}\left[S(0,0) \quad S(x-x', t-t')\, e^{-\beta H} \right]$$

Now insert $1 = e^{-\beta H}e^{\beta H}$ between the two S operators and replace

$$e^{\beta H}\, S(x-x', t-t')\, e^{-\beta H} = S(x-x', t-t'-i\beta)$$

This numerator term can now be written

$$\operatorname{tr}\left[S(0,0)\ e^{-\beta H}\ S(x-x', t-t'-i\beta)\right] = \operatorname{tr}\left[S(x-x', t-t'-i\beta)\, S(0,0)\, e^{-\beta H}\right]$$

so that the commutator becomes

$$\langle [S(\vec{x},t), S(\vec{x}',t')] \rangle = \langle [S(x-x', t-t') - S(x-x', t-t'-i\beta)] \, S(0,0) \rangle$$

Since

$$C(k,\omega) = \int dt \, d^3x \; e^{i\omega t} e^{-i\vec{k}\cdot\vec{x}} \langle S(x,t) S(0,0) \rangle$$

the Fourier transform of χ'' becomes

$$\chi'' = \frac{1}{2\hbar} \left(1 - e^{-\beta\hbar\omega}\right) C(\vec{k},\omega)$$

I have inserted factors of $\hbar$ in the correct places. The $\hbar \to 0$ limit of this expressive gives the classical mechanics formula for $\chi''(\vec{k},\omega)$ presented above.