Week 9 - Classical fluctuation dissipation theorem

I. LANGEVIN EQUATION

So far we always assumed that whatever particles we have in our statistical mechanical systems, they are somehow in equilibrium. But how is this equilibrium obtained? One answer is Langevin noise. We can consider our system as being subject to a random force, which pushes the particles around to produce just the right amount of fluctuations. Does this make sense? As a first example consider just a single particle in 1d, with mass \( m \) in a random noise field \( \eta(t) \) which has some distribution, probably Gaussian, but in particular, is noncorrelated in time:

\[
\langle \eta(t)\eta(t') \rangle = \delta(t-t')(\eta^2) \tag{1}
\]

Let’s write the equation of motion for this particle, with initial momentum \( p_0 = 0 \):

\[
m\ddot{x} = \eta(t) \tag{2}
\]

which we can solve with:

\[
m\dot{x} = \int_0^t dt \eta(t) \tag{3}
\]

On average this is zero, but what about the width?

\[
\langle (m\dot{x})^2 \rangle = \int_0^t dt \int_0^t dt' \langle \eta(t)\eta(t') \rangle = \int_0^t dt \langle \eta^2 \rangle = \langle \eta^2 \rangle t \tag{4}
\]

not good... This diverges at long times, which means that our particle actually has more energy than the expectation from statistical mechanics theory:

\[
\langle p^2/2m \rangle = T/2. \tag{5}
\]

How can we resolve this? In fact, what did we forget? If the particle at hand is moving through a random potential, that potential is fully random only in the rest frame. If so, it is probably going to be also providing a drag force on a moving particle. Therefore we need to modify the equation of motion by a friction:

\[
m\ddot{x} + \gamma \dot{x} = \eta(t) \tag{6}
\]

This is called the Langevin equation.

To approach this problem we need to go to Fourier space. First, let’s convert the noise correlator into a statement about Fourier coefficients:

\[
\langle \eta_\omega \eta_{\omega'} \rangle = \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' e^{i\omega t} e^{i\omega' t'} \langle \eta(t)\eta(t') \rangle
\]

\[
= \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} dt' e^{i\omega t} e^{i\omega' t'} \delta(t-t') \langle \eta^2 \rangle
\]

\[
= 2\pi \delta(\omega + \omega') \langle \eta^2 \rangle. \tag{7}
\]

Now, the equation of motion is:

\[
(-m\omega^2 - i\gamma \omega) x_\omega = \eta_\omega. \tag{8}
\]

And we are interested in the square of the velocity:

\[
\langle (\dot{x}(t))^2 \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{-i\omega e^{-i\omega t}}{(-m\omega^2 - i\gamma \omega)} \frac{-i\omega' e^{-i\omega' t}}{(-m\omega'^2 - i\gamma \omega')} \langle \eta_\omega \eta_{\omega'} \rangle. \tag{9}
\]
Putting in the delta function, and carrying out one frequency integration we get:

\[ \langle \dot{x}(t)^2 \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\omega^2 \langle \eta^2 \rangle}{m^2 \omega^4 + \gamma^2 \omega^2} \]

with the Fourier factors neatly canceling each other. This reduces to a simple contour integral,

\[ = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{\langle \eta^2 \rangle}{m^2 (\omega + i\gamma/m)(\omega - i\gamma/m)} \]

which picks a pole at \( \omega = i\gamma/m \), and gives:

\[ \langle \dot{x}^2 \rangle = \frac{\langle \eta^2 \rangle}{2m\gamma} \]

finite at least! This should now be compared with what we know from the equipartition theorem, and we get:

\[ \frac{1}{2}m\dot{x}^2 = \frac{\langle \eta^2 \rangle}{4\gamma} = \frac{1}{2}T \]

This translates to a general, and rather profound, result:

\[ \langle \eta^2 \rangle = 2\gamma T \]

The variance of the fluctuating force is proportional to the temperature times the friction.

The relation between \( \langle \eta^2 \rangle \) and \( \gamma \) implies that the damping and the random force are two aspects of the same thing. In the case of a smoke particle diffusing through a gas, this makes perfect sense: on the one hand the gas particles randomly collide with the smoke particle, giving a random force. On the other hand, when the smoke particle moves relative to the rest frame of the gas, it sees a head wind, which results in damping. The validity of the relationship (14), however, goes well beyond the scope of the smoke narrative.

### II. RESPONSE FUNCTION

To be able to generalize the noise vs. dissipation results, we need to formally define some physical properties of a system. First, the response function, \( \chi(t) \).

If we apply a force \( F(t) \) to our particle, we can write the EOM as:

\[ m\ddot{x} + \gamma \dot{x} = F(t) \]

Now, the particle’s position at time \( t \) will depend on the force at all past times. Furthermore, that dependence should be linear. Therefore we should be able to define a response function, \( \chi(t) \), such that:

\[ x(t) = \int_{-\infty}^{t} dt' F(t') \chi(t - t') \]

so \( \chi(t - t') \) gives the weight that the force \( F \) at \( t' \) has on the location of the particle at time \( t \). Again, it is best viewed in Fourier space. But we must be careful: since response is causal, \( \chi(t - t') \) is only defined for a positive argument, \( t > t' \). So:

\[ \chi(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \chi_\omega \]

but:

\[ \chi_\omega = \int_{0}^{\infty} dt e^{i\omega t} \chi(t) \]
With this definition we write:

\[ x_\omega = \int_0^\infty dt' F(t-t') \chi(t) = \int_0^\infty dt' \int_0^\infty \frac{d\omega'}{2\pi} F_{\omega'} e^{-i\omega'(t-t')} \chi(t'). \]  

(19)

Doing the \( t \) integral first forces \( \omega' = \omega \):

\[ x_\omega = \int_0^\infty dt' 2\pi F_{\omega} e^{i\omega t'} \chi(t') = F_{\omega} \chi_{\omega} \]  

(20)

After this careful prep work, we can just read off what \( \chi \) is:

\[ (-\omega^2 m - i\omega\gamma)x_\omega = F_{\omega} \]  

(21)

and:

\[ \chi_{\omega} = \frac{1}{-\omega^2 m - i\omega\gamma}. \]  

(22)

In some cases (for instance, in magnetic systems) this response is also called a susceptibility.

Let’s look at it very briefly. Write:

\[ \chi_{\omega} = \chi'_{\omega} + i\chi''_{\omega} \]  

(23)

and we see that the real part is:

\[ \chi'_{\omega} = \frac{-m}{m^2 \omega^2 + \gamma^2} \]  

(24)

this is the inductive part - it has no dissipation in it, which means that it creates a motion that has \( \dot{x} \) lagging by \( \pi/2 \) behind the force. The dissipation appears prominently in \( \chi'' \):

\[ \chi''_{\omega} = \frac{\gamma/\omega}{m^2 \omega^2 + \gamma^2} \]  

(25)

If there was no dissipation, this piece would vanish.

### III. CORRELATIONS

In addition to the response, which shows dissipation in the imaginary piece, it is natural to ask what are the correlations between \( x(t) \) at different times:

\[ \langle x(t) x(0) \rangle \]  

(26)

where the averaging is over thermal noise, which should be construed as an average over all times:

\[ \frac{1}{T_{\text{total}}} \int_{-T_{\text{total}}/2}^{T_{\text{total}}/2} dt' x(t' + t) x(t'). \]  

(27)

The FT of the correlation as a function of \( \omega \) is:

\[ C_{\omega} = \int dt \langle x(t) x(0) \rangle e^{i\omega t} \]  

(28)

Let’s massage this into containing \( x_\omega \):

\[ C_{\omega} = \int dt e^{i\omega t} \frac{1}{T_{\text{total}}} \int_{-T_{\text{total}}/2}^{T_{\text{total}}/2} dt' \langle x(t' + t) x(t') \rangle \]  

(29)
which, by Parseval’s identity is:

\[
\int dt e^{i\omega t} \frac{1}{T_{\text{total}}} \int \frac{d\omega'}{2\pi} \langle x_{\omega} x_{-\omega} \rangle e^{-i\omega't} = \frac{1}{T_{\text{total}}} \langle x_{\omega} x_{-\omega} \rangle
\]  
(30)

This doesn’t look like it is making sense, but consider what \( x_{\omega} \) is when we have Liouville noise - it is:

\[
x_{\omega} = \chi_{\omega} \eta_{\omega}
\]  
(31)

and therefore:

\[
\langle x_{\omega} x_{-\omega} \rangle = \chi_{\omega} \chi_{-\omega} \langle \eta_{\omega} \eta_{-\omega} \rangle
\]

\[
\chi_{\omega} \chi_{-\omega} \langle \eta_{\omega}^2 \rangle 2\pi \delta(\omega - \omega) = \chi_{\omega} \chi_{-\omega} \langle \eta_{\omega}^2 \rangle T_{\text{total}}
\]

where we used the fact that \( \delta(\omega) = \frac{1}{d\omega} \), and that the measure for \( \omega \) is: \( d\omega = 2\pi/T_{\text{total}} \). Thus:

\[
C_{\omega} = \chi_{\omega} \chi_{-\omega} \langle \eta_{\omega}^2 \rangle
\]  
(33)

finite!

**IV. FLUCTUATION DISSIPATION THEOREM**

Eq. (33), using the identity (14) can be cast in the following form:

\[
C_{\omega} = \chi_{\omega} \chi_{-\omega} 2\gamma T
\]  
(34)

Putting in \( \chi = 1/(-m\omega^2 - i\gamma \omega) \) we see that:

\[
\chi_{\omega} \chi_{-\omega} \gamma = \chi'' \omega.
\]  
(35)

This, you’ll convince yourself in the problem set, is generally true for a quantum system. And we get:

\[
C_{\omega} = \chi'' \omega 2T/\omega = 2T/\omega \Im \chi_{\omega}.
\]  
(36)

This is the fluctuation-dissipation theorem. It is a deep connection between the fluctuations of any variable in your system, and the dissipation that time derivatives of that parameter show.

One very important example of this result is the Johnson-Nyquist noise. In a circuit with resistor R in series with a battery as well as other inductors or capacitors, the voltage on the resistor will fluctuate as:

\[
\langle (\Delta V)^2 \rangle_{\omega} = 2RT
\]  
(37)

(note that in steady state there is no current in a circuit like that since the capacitors get charged and produce a disconnect). This allows for very good circuit thermometry, especially when this relation is generalized into the quantum realm.