PH4211 Statistical Mechanics

Problem Sheet 5 — Answers

1 A random quantity has an exponential autocorrelation function $G(t) = G(0)e^{-\gamma t}$. Calculate its correlation time using the usual definition.

The correlation time is the 'width' of the correlation function – the area divided by the height. Thus the definition

$$\tau_\mathrm{c} = \frac{1}{G(0)} \int_0^\infty G(t)\,\mathrm{d}t\,.$$

So for the exponential correlation function

$$\begin{aligned}\tau_\mathrm{c} &= \int_0^\infty e^{-\gamma t}\,\mathrm{d}t \\ &= \left.\frac{e^{-\gamma t}}{-\gamma}\right|_0^\infty = \frac{1}{\gamma}\,.\end{aligned}$$

The correlation time is simply $1/\gamma$ – the time constant of the exponential.

2 Show that the autocorrelation function of a periodically varying quantity $m(t) = m\cos\omega t$ is given by

$$G(t) = \frac{m^2}{2}\cos\omega t\,.$$

Show that the autocorrelation function is independent of the *phase* of $m(t)$. In other words, show that if $m(t) = m\cos(\omega t + \varphi)$, then $G(t)$ is independent of φ.

The autocorrelation function is defined by

$$G(t) = \langle m(\tau)m(\tau + t)\rangle\,.$$

It is convenient here to regard the average as a time average. That is, we average over τ so that $G(t)$ is calculated as

$$G(t) = \frac{1}{2T}\int_{-T}^{T} m(\tau)m(\tau + t)\,\mathrm{d}\tau\,.$$

But actually we don't need to do any integration, as we shall see. We star from $m(t) = m\cos\omega t$, so that

$$\begin{aligned}G(t) &= \langle m(\tau)m(\tau + t)\rangle \\ &= \langle m\cos(\omega\tau)\, m\cos\omega(\tau + t)\rangle.\end{aligned}$$

We use the trig identity $\cos(x + y) = \cos x\cos y - \sin x\sin y$, so that

$$G(t) = \langle m^2\cos^2\omega\tau\cos\omega t\rangle + \langle m^2\cos\omega\tau\sin\omega\tau\sin\omega t\rangle\,.$$

The average is evaluated over τ, thus

$$G(t) = m^2\cos\omega t\langle\cos^2\omega\tau\rangle + m^2\sin\omega t\langle\cos\omega\tau\sin\omega\tau\rangle\,.$$

The average of cos^2 is ½; the function varies smoothly between 0 and 1. The average of cos sin is zero; this function varies smoothly between –1 and +1. Thus we conclude that

$$G(t)=\frac{m^2}{2}\cos\omega t$$

as required.

Now consider the case $m(t)=m\cos(\omega t+\varphi)$. Then

$$\begin{aligned}G(t)&=\langle m(\tau)m(\tau+t)\rangle\\&=\langle m\cos(\omega\tau+\varphi)m\cos(\omega\tau+\varphi+\omega t)\rangle.\end{aligned}$$

We use the same trig identity to obtain

$$G(t)=\langle m^2\cos^2(\omega\tau+\varphi)\cos\omega t\rangle+\langle m^2\cos(\omega\tau+\varphi)\sin(\omega\tau+\varphi)\sin\omega t\rangle.$$

The average is evaluated over τ, thus

$$G(t)=m^2\cos\omega t\langle\cos^2(\omega\tau+\varphi)\rangle+m^2\sin\omega t\langle\cos(\omega\tau+\varphi)\sin(\omega\tau+\varphi)\rangle.$$

Then, once again, the average of cos^2 is ½ and the average of cos sin is zero. And so in this case also we obtain

$$G(t)=\frac{m^2}{2}\cos\omega t\ ;$$

this shows that $G(t)$ is independent of φ as required.

3 The dynamical response function $X(t)$ must vanish at zero times, as shown in Fig. 5.13. What is the physical explanation of this? What is the consequence for the step response function $\Phi(t)$? Is this compatible with an exponentially decaying $\Phi(t)$?

The step response function $\Phi(t)$ is proportional to the autocorrelation function of the response variable

$$\Phi(t)\propto\langle M(0)M(t)\rangle,$$

from the Onsager hypothesis or the linear response derivation. Since, certainly in the classical case, $M(0)$ and $M(t)$ commute, we may swap these around so that

$$\Phi(t)=\Phi(-t).$$

Thus $\Phi(t)$ is an even function and its odd derivatives must vanish at $t = 0$. And then since $X(t)$ is the first derivative of $\Phi(t)$, it follows that $X(0) = 0$ as required.

If the odd derivatives of $\Phi(t)$ vanish at the origin, this is clearly incompatible with an exponential decay. More precisely $\Phi(t)$ cannot decay exponentially *in the vicinity of* $t = 0$; it can elsewhere.

4 In Section 5.3 we examined the form of the dynamical susceptibility $\chi(\omega)$ that followed from the assumption that the step response function $\Phi(t)$ decayed exponentially. In this question consider a step response function that decays with a gaussian profile, $\Phi(t)=\chi_0e^{-t^2/2\tau^2}$. Evaluate the real and imaginary parts of the dynamical susceptibility and plot them as a function of frequency. The real part of the susceptibility is difficult to evaluate without a symbolic mathematics system such as

Mathematica. Compare and discuss the differences and similarities between this susceptibility and that deduced from the exponential step response function (Debye susceptibility).

The response function $X(t)$ is given by minus the derivative of $\Phi(t)$, thus

$$X(t) = -\frac{\mathrm{d}}{\mathrm{d}t}\chi_0 e^{-t^2/2\tau^2}$$

$$= \chi_0 \frac{t}{\tau^2} e^{-t^2/2\tau^2}.$$

The dynamical susceptibility is the Fourier transform of this

$$\chi(\omega) = \int_{-\infty}^{\infty} X(t) e^{\mathrm{i}\omega t} \mathrm{d}t$$

so that

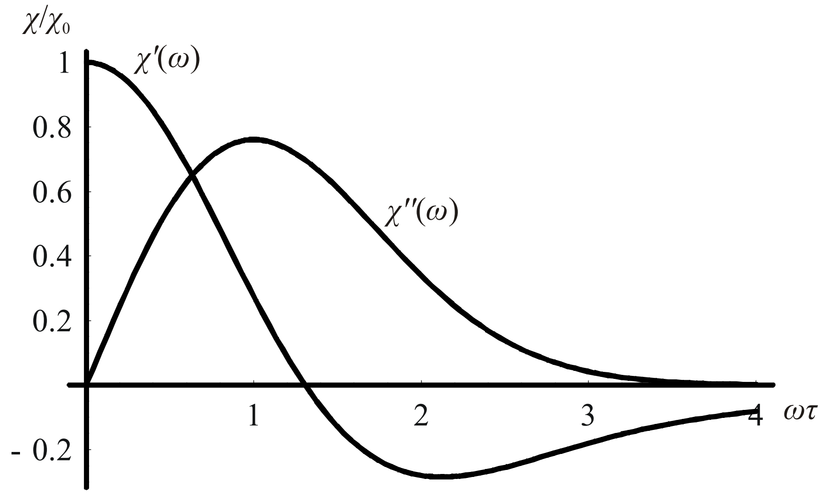
$$\chi(\omega) = \frac{\chi_0}{\tau^2} \int_{-\infty}^{\infty} t e^{-t^2/2\tau^2} e^{\mathrm{i}\omega t} \mathrm{d}t \, .$$

Upon integration we obtain the real and imaginary parts as

$$\chi'(\omega) = \chi_0 \left\{ 1 - \sqrt{\frac{\pi}{2}} \omega\tau e^{-\omega^2\tau^2/2} \operatorname{erfi} \frac{\omega\tau}{\sqrt{2}} \right\}$$

$$\chi''(\omega) = \chi_0 \sqrt{\frac{\pi}{2}} \omega\tau e^{-\omega^2\tau^2/2}.$$

These are plotted in the figure.



The imaginary part of the susceptibility is always positive, as required by energy considerations. In this case the real part of the susceptibility goes negative. This is in contrast to that of the Debye susceptibility, that remains positive at all frequencies.

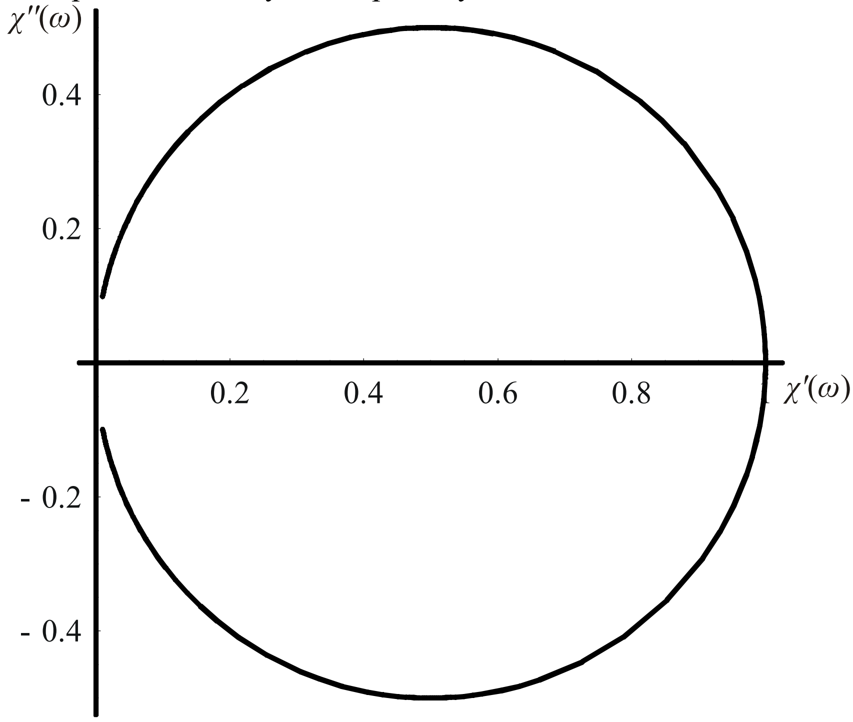
5 The Debye form for the dynamical susceptibility is

$$\chi'(\omega) = \chi_0 \frac{1}{1+\omega^2\tau^2}$$

$$\chi''(\omega) = \chi_0 \frac{\omega\tau}{1+\omega^2\tau^2}.$$

Plot the real part against the imaginary part and show that the figure corresponds to a semicircle. This is known as a Cole-Cole plot.

The Cole-Cole plot of the Debye susceptibility is shown below.



The upper half circle corresponds to positive frequencies and the lower half corresponds to negative frequencies.

The real and imaginary parts pf the Debye susceptibility are seen to satisfy the equation

$$\left(\frac{\chi''}{\chi_0}\right)^2 + \left(\frac{\chi'}{\chi_0} - \frac{1}{2}\right)^2 = \left(\frac{1}{2}\right)^2.$$

This is corresponds to a circle of radius ½ centred on $\chi'/\chi_0 = 1/2$.

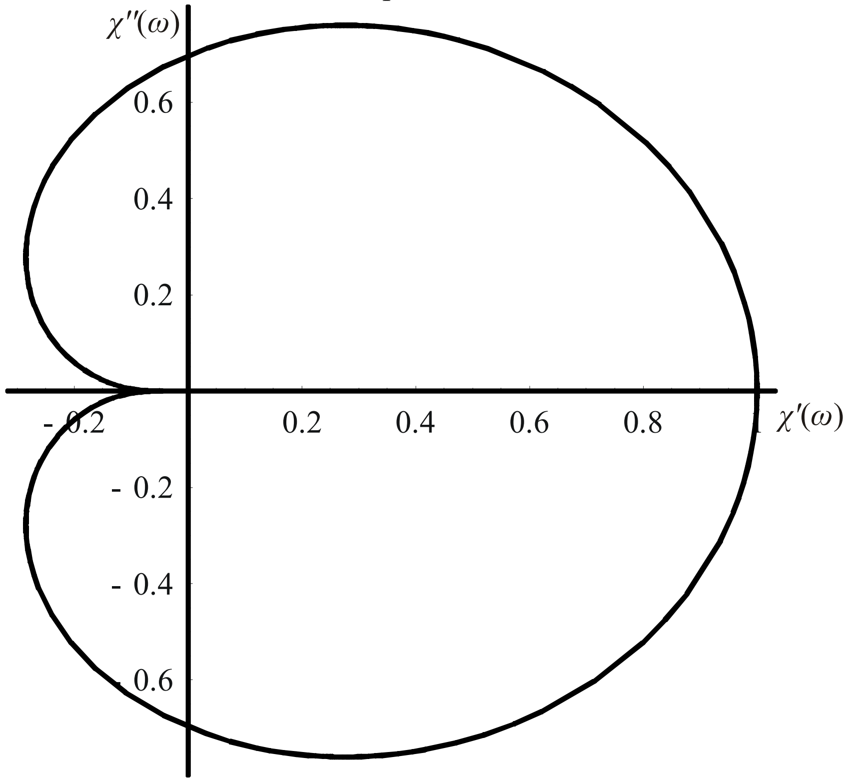
6 Plot the Cole-Cole plot (Problem 5.5) for the dynamical susceptibility considered in Problem 5.4. How does it differ from that of the Debye susceptibility.

In Problem 5.4 we obtained the expressions for the real and the imaginary parts of the dynamical susceptibility

$$\chi'(\omega) = \chi_0 \left\{1 - \sqrt{\frac{\pi}{2}}\omega\tau e^{-\omega^2\tau^2/2} \operatorname{erfi}\frac{\omega\tau}{\sqrt{2}}\right\}$$

$$\chi''(\omega) = \chi_0 \sqrt{\frac{\pi}{2}}\omega\tau e^{-\omega^2\tau^2/2}.$$

From these we can make the Cole-Cole plot:



The main difference from the Debye form is that this curve passes to the left of the y axis (high frequencies), where the real part of the susceptibility becomes negative. Since in the high frequency limit the real and imaginary parts of the susceptibility must both vanish, this gives the cardioid shape to the plot.

7 The full quantum-mechanical calculation of the Johnson noise of a resistor gives

$$\left\langle v^2 \right\rangle_{\Delta f} = 4R\frac{hf}{e^{hf/kT}-1}\Delta f \ .$$

Show that this reduces to the classical Nyquist expression at low frequencies. At what frequency will there start to be serious deviations from the Nyquist value? Estimate the value of this frequency.

At low frequencies such that $hf \ll kT$ we can expand the exponential so that

$$\begin{aligned}\left\langle v^2 \right\rangle_{\Delta f} &= 4R\frac{hf}{1+hf/kT+\ldots-1}\Delta f \\ &= 4R\frac{hf}{hf/kT+\ldots}\Delta f\end{aligned}$$

and in the low frequency limit the hf cancels, giving

$$\left\langle v^2 \right\rangle_{\Delta f} = 4kTR\Delta f \ ,$$

the classical Nyquist expression.

For the Nyquist expression to be valid we require the frequency to satisfy $f \ll kT/h$, so at room temperature ($T \sim 300\text{K}$) this means

$$f << \frac{1.4\times10^{-23}\times300}{6.6\times10^{-34}} = 6.4\times10^{12}\,\mathrm{Hz}.$$

8 Show that for the Debye susceptibility, the relation

$$\chi_0 = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\chi''(\omega)}{\omega}\,\mathrm{d}\omega$$

holds. Demonstrate that χ'' vanishes sufficiently fast at $\omega = 0$ so there is no pole in the integral and there is thus no need to take the principal part of the integral in the Kramers-Kronig relations.

In the Debye case

$$\chi''(\omega) = \chi_0\frac{\omega\tau}{1+\omega^2\tau^2}$$

so that the integrand is

$$\frac{\chi''(\omega)}{\omega} = \chi_0\frac{\tau}{1+\omega^2\tau^2} \quad .$$

The ω in the denominator has been cancelled by the ω in the numerator. Thus there is no pole in the integral.

We wish to evaluate the integral

$$I = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\chi''(\omega)}{\omega}\,\mathrm{d}\omega = \chi_0\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\tau}{1+\omega^2\tau^2}\,\mathrm{d}\omega.$$

We can remove the τ by changing variables to $x = \omega\tau$, so that $\mathrm{d}\omega = \mathrm{d}x/\tau$, and

$$I = \chi_0\frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\mathrm{d}x}{1+x^2} \quad .$$

The integral is standard; its value is π. Thus we have shown that $I = \chi_0$; we have demonstrated that the Kramers-Krönig sum rule holds in the Debye case.

5.9 In Section 5.3.6 we considered an electrical analogue of the Langevin Equation based on a circuit comprising an inductor and a resistor. In this problem we shall examine a different analogue: a circuit of a capacitor and a resistor. Show that the equation analogous to the Langevin equation, in this case, is

$$C\frac{\mathrm{d}V(t)}{\mathrm{d}t} + \frac{1}{R}V(t) = I(t).$$

Hence show that the fluctuation-dissipation result relates the resistance to the current fluctuations through

$$\frac{1}{R} = \frac{1}{2kT}\int_{-\infty}^{\infty}\langle I(0)I(t)\rangle\,\mathrm{d}t\,.$$