E7020+E7488: Oscillators in FDT

Submitted by: Oren Rosenblatt, Michael Chapsky, Nimrod Cohen

Question

Consider a mass M on a harmonic oscillator of frequency Ω ,The oscillator experiences dumping with coefficient η, and external force $f(t)$. The system is at temperature T.

1. Write the generalized susceptibility that describes the response of x to the driving by the external force $f(t)$.
2. Using FD relations find power spectrum for x and for v.
3. Find the general expression for the autocorrelation function $\langle v(t+\tau)v(t)\rangle$ (in the integral form), find the exact expression for high temperatures for both the classical case, and quantum case. How is it consistent with the canonical result ?
4. Evaluate the driving force power spectrum in the high temperature limit.
   Hint: $v(t) = v(0)e^{-t/\tau} + e^{-t/\tau}\int_0^t e^{u/\tau} f(u)du$
5. Find the fluctuations in the limit $\gamma \to 0$ the fluctuations $\left\langle v^2\right\rangle$ and $\left\langle x^2\right\rangle$ (quantum and classical). Show consistency with the canonical results.

Solution

1. The equation of motion, defining $\gamma = \frac{\eta}{M}$, (from now on we will use this notation for convenience):

$$\ddot{x} + \gamma\dot{x} + \Omega^2 x = \frac{1}{M} f(t)$$

Therefore the response of x to the external force is given by the equation:

$$x_\omega = \frac{1}{M}\cdot\frac{1}{\Omega^2 - \omega^2 - i\gamma\omega}\cdot f_\omega$$

and the susceptibility itself is:

$$\chi = \frac{1}{M}\cdot\frac{1}{\Omega^2 - \omega^2 - i\gamma\omega}$$

2. FD Relations states that ($\tilde{C}(\omega)$ relates to power spectrum of x unless otherwise stated by an index):

$$\frac{\mathrm{Im}\left(\chi(\omega)\right)}{\omega} = \frac{1}{\hbar\omega}\tanh\left(\frac{\hbar\omega}{2K_bT}\right)\cdot\tilde{C}(\omega)$$

it is then straightforward to get:

$$\tilde{C}^{xx}(\omega) = \hbar\omega\cdot\coth\left(\frac{\hbar\omega}{2K_bT}\right)\cdot\frac{\mathrm{Im}\left[\chi(\omega)\right]}{\omega} = \frac{1}{M}\cdot\frac{\hbar\omega\gamma}{\left(\omega^2-\Omega^2\right)^2+\gamma^2\omega^2}\coth\left(\frac{\hbar\omega}{2K_bT}\right)$$

since $v_\omega = -i\omega x_\omega$, in the same way we get (can also be obtained by Winner-Kintchin Theorem):

$$\tilde{C}^{vv}(\omega) = \frac{1}{M}\cdot\frac{\hbar\omega^3\gamma}{\left(\omega^2-\Omega^2\right)^2+\gamma^2\omega^2}\coth\left(\frac{\hbar\omega}{2K_bT}\right)$$

3. Autocorrelation function is $C(\tau) = \langle v(t+\tau)v(t)\rangle$ and since $C(\tau)$ is the inverse Fourier Transform of $\tilde{C}(\omega)$ we get:

$$C^{vv}(\tau) = \int\limits_{-\infty}^{+\infty} \frac{\hbar\omega^3}{M} \frac{\gamma}{\left(\omega^2 - \Omega^2\right)^2 + \omega^2\gamma^2} \exp\left(i\omega\tau\right) \coth\left(\frac{\hbar\omega}{2K_bT}\right) \frac{d\omega}{2\pi}$$

in the limit of high temperatures ($\Omega \to 0$) we get $\coth x \to \frac{1}{x}$ and the correlation integral becomes:

$$C^{vv}(\tau) = \int\limits_{-\infty}^{+\infty} \frac{2K_bT}{M} \frac{\gamma \exp\left(i\omega\tau\right)}{\omega^2 + \gamma^2} \frac{d\omega}{2\pi}$$

and then using contour integration and residue theorem we fonally get:

$$C^{vv}(\tau) = \frac{K_bT}{M} \exp\left(-\gamma\tau\right)$$

so we got the brownian particle as a result.
the result can also be compared to the canonical result by using $\left\langle v^2 \right\rangle = C(0) = \frac{K_bT}{M}$, and therefore we get the consistency with equipartition:

$$\left\langle \frac{1}{2}Mv^2 \right\rangle = \frac{1}{2}K_bT$$

4. The formal solution of Langevin equation in the high temperature limit ($\Omega \to 0$) is

$$v(t) = v(0)e^{-t/\tau} + e^{-t/\tau} \int_0^t e^{u/\tau} f(u) du$$

Multiplying both sides of the equation by the random force yields

$$v(t)f(t) = v(0)f(t)e^{-t/\tau} + e^{-t/\tau} f(t) \int_0^t e^{u/\tau} f(u) du$$

This is nothing but the momentary power spectrum. The exception value of the power is

$$\langle v(t)f(t)\rangle = v(0)\langle f(t)\rangle e^{-t/\tau} + e^{-t/\tau} \int_0^t e^{u/\tau} \langle f(t)f(u)\rangle du$$

The first term in the right wing tends to zero since the average of a random force is zero. In order to deal with the second term we make the following substitution

$$x = t - u$$

so the equation takes the form

$$\langle v(t)f(t)\rangle = -\int_t^0 e^{-x/\tau} k(x) dx$$

where

$$k(x) \equiv \langle f(t-x)f(t)\rangle$$

When $t < \tau$ a rough approximation can be made - $e^{-x/\tau} \approx 1$ and for the other case, $t > \tau$, $k = 0$ so we can change the boundaries of the integral to the whole space and divide by two (because of the parity of integrad).

$$\langle v(t)f(t)\rangle = -\int_t^0 e^{-x/\tau}k(x)dx = \frac{1}{2}\int_{-t}^{t} e^{-|x|/\tau}k(x)dx \approx \frac{1}{2}\int_{-\infty}^{\infty} k(x)dx = \frac{C}{2}$$

The next step is to evaluate C from thermodynamic considerations. Squaring the formal solution of $v(t)$ and taking its exception value gives the following equation

$$< v^2(t) >= v^2(0)e^{-2t/\tau} + C\frac{\tau}{2}\left(1 - e^{-2t/\tau}\right)$$

in the limit of $t \gg \tau$ last equation becomes

$$< v^2 >= C\frac{\tau}{2}$$

On the other side, from the equipartition law we get

$$< v^2 >= \frac{kT}{m}$$

and equating the last two equation we find

$$C = \frac{2k_B T}{m\tau}$$

substituting it back to the driving force power spectrum expression gives

$$\langle v(t)f(t)\rangle = \frac{k_B T}{m\tau} = \frac{k_B T\gamma}{m}$$

5.

For the limit $\gamma \to 0$ the expression for $\tilde{C}^{vv}(\omega)$ is (using the lorentzian definition of delta):

$$\frac{\tilde{C}^{vv}(\omega)}{\coth\left(\frac{\hbar\omega}{2K_bT}\right)} = \frac{\hbar\omega}{M}\frac{\gamma}{\gamma^2 + \left(\omega - \frac{\Omega^2}{\omega}\right)^2} \to \frac{\hbar\omega}{M}\pi\delta(\omega - \frac{\Omega^2}{\omega})$$

since the delta function is of composite function we use the identity

$$\delta(f(x)) = \frac{1}{|f‘(x_i)|}\sum\delta(x - x_i)$$

where X_i are the solutions of $f(x) = 0$
we therefore get:

$$\delta(\omega - \frac{\Omega^2}{\omega}) = \frac{1}{2}\left(\delta(\omega + \Omega) + \delta(\omega - \Omega)\right)$$

and the fluctuations becomes

$$C^{vv}(\tau = 0) = \int\limits_{-\infty}^{+\infty}\tilde{C}^{vv}(\omega)\frac{d\omega}{2\pi} = \int\limits_{-\infty}^{+\infty}\frac{\pi\hbar\omega}{4\pi M}\coth\left(\frac{\hbar\omega}{2K_bT}\right)(\delta(\omega + \Omega) + \delta(\omega - \Omega))d\omega$$

calculating the integral gives the result (quantum case):

$$\langle v^2\rangle = \frac{\hbar\Omega}{2M}\coth\left(\frac{\hbar\Omega}{2K_bT}\right)$$

to check our result we look at the Hamiltonian of harmonic oscillator $\hat{H} = \left(a^\dagger a + \frac{1}{2}\right)\hbar\Omega$ and since the bosonic occupation for temperature T is given by :

$$N = \left\langle a^\dagger a \right\rangle = \frac{1}{\exp\left(\frac{\hbar\Omega}{K_b T}\right) - 1}$$

we get for the harmonic oscillator (for writing convinience $\beta = 1/K_b T$):

$$E = \left(\frac{1}{\exp\left(\beta\hbar\Omega\right) - 1} + \frac{1}{2}\right)\hbar\Omega = \frac{\hbar\Omega}{2}\frac{\exp\left(\beta\hbar\Omega/2\right) + 1}{\exp\left(\beta\hbar\Omega/2\right) - 1} = \frac{1}{2}\hbar\Omega\coth\left(\frac{\hbar\Omega}{2K_b T}\right)$$

now if we take into account that $\frac{1}{2}M\left\langle v^2\right\rangle = \frac{1}{2}E$, we see that the result is consistent with the quantum case solution and we have the equality:

$$\frac{1}{2}M\left\langle v^2\right\rangle = \frac{1}{4}\hbar\Omega\coth\left(\frac{\hbar\Omega}{2K_b T}\right)$$

For the classical case, we take $\hbar \to 0$ and we get (same as in the previous section) :

$$\frac{1}{2}M\left\langle v^2\right\rangle = \frac{2K_b T}{4}\frac{\hbar\Omega}{\hbar\Omega} = \frac{K_b T}{2}$$

since the relations between power spectra of v and x is $\tilde{C}^{vv}(\omega) = \omega^2\tilde{C}^{xx}(\omega)$ we then have the fluctuations of x:

$$C^{xx}(0) = \int \frac{d\omega}{4\pi}\frac{\hbar\pi}{\omega M}\coth\left(\frac{\hbar\omega}{2K_b T}\right)\cdot\left(\delta(\omega - \Omega) + \delta(\omega + \Omega)\right)$$

calculating the integral we get:

$$\left\langle x^2\right\rangle = \frac{\hbar}{2M\Omega}\coth\left(\frac{\hbar\Omega}{2K_b T}\right)\underset{classical}{\rightarrow}\frac{K_b T}{M\Omega^2}$$

which is consistent with the equipartition :

$$\frac{1}{2}M\Omega^2\left\langle x^2\right\rangle = \frac{K_b T}{2}$$