

E7020+E7488: Oscillators in FDT

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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. Find the fluctuations in the limit $\gamma \rightarrow 0$ the fluctuations $\langle v^2 \rangle$ and $\langle x^2 \rangle$ (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):

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

it is then straightforward to get:

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

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

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

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:

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

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

$$C^{vv}(\tau) = \int_{-\infty}^{+\infty} \frac{2K_b T}{M} \frac{\gamma \exp(i\omega\tau)}{\omega^2 + \gamma^2} \frac{d\omega}{2\pi}$$

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

$$C^{vv}(\tau) = \frac{K_b T}{M} \exp(-\gamma\tau)$$

so we got the brownian particle as a result.

the result can also be compared to the canonical result by using $\langle v^2 \rangle = C(0) = \frac{K_b T}{M}$, and therefore we get the consistency with equipartition:

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

4.

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

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

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:

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

and the fluctuations becomes

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

calculating the integral gives the result (quantum case):

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

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

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

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

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

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

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

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

$$\frac{1}{2}M\langle v^2 \rangle = \frac{2K_bT}{4} \frac{\hbar\Omega}{\hbar\Omega} = \frac{K_bT}{2}$$

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 :

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

calculating the integral we get:

$$\langle x^2 \rangle = \frac{\hbar}{2M\Omega} \coth\left(\frac{\hbar\Omega}{2K_bT}\right) \xrightarrow{\text{classical}} \frac{K_bT}{M\Omega^2}$$

which is consistent with the equipartition :

$$\frac{1}{2}M\Omega^2\langle x^2 \rangle = \frac{K_bT}{2}$$