

E8032: Sub diffusion of Brownian particle

Submitted by: Michael Chapsky

Question

The motion of a brownian particle in 1D is given by the Hamiltonian:

$$H_{Total}(x, p; A(t)) = \frac{1}{2m}(p - A(t))^2 + H_{Bath}(x)$$

and the equation of motion is:

$$m \frac{\partial \langle v \rangle}{\partial t} = -\eta \langle v \rangle + f(t)$$

1. Define $f(t)$ from $A(t)$.
2. What is the generalised susceptibility χ . (of v driven by A)
3. Find the power spectrum $\tilde{C}(\omega)$ of the velocity v .
4. Find the explicit expression for the correlation function $C(\tau)$ in the limit of high and low temperatures.

For the following questions assume $T = 0$.

5. Find the coefficient C_0 in $C(\tau) \sim -C_0/\tau^2$.
6. Given the definition $S(t) = \langle (x(t) - x(0))^2 \rangle$, Find an expression for $\frac{dS(t)}{dt}$, using the correlation function $C(\tau)$.
7. Given $S(t_0) = S_0$, find $S(t)$ for $t > t_0$.

Solution

1. Hamilton equations give:

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{1}{m}(p - A)$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -\frac{\partial H_{bath}}{\partial x}$$

They give a straightforward solution (equation of motion):

$$m \frac{\partial \dot{x}}{\partial t} = -\frac{\partial H_{bath}}{\partial x} - \frac{\partial A}{\partial t}$$

The two terms on the right can then be easily identified (taking an ensemble average):

$$f(t) = -\frac{\partial A}{\partial t}$$

$$\eta = \frac{\partial H_{bath}}{\partial x}$$

2. Fourier transforming the equation of motion results in:

$$(\eta - i\omega m) v_\omega = i\omega A_\omega$$

and if we define $\tau_\eta = m/\eta$ we get the we get:

$$\chi(\omega) = \frac{1}{\eta} \frac{i\omega}{1 - i\omega\tau_\eta}$$

3. The FD relations are:

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

and from (2) it is known that $\frac{\text{Im}[\chi]}{\omega} = \frac{1}{\eta} \frac{1}{1+(\omega\tau_\eta)^2}$ we therefore get the power spectrum of v to be:

$$\tilde{C}(\omega) = \frac{1}{\eta} \frac{\hbar\omega}{1 + (\omega\tau_\eta)^2} \coth\left(\frac{\hbar\omega}{2K_B T}\right)$$

4. In order to obtain the high and low temperature limits we note the behaviour of $\coth(x)$ at the requested limits:

$$\coth(x) \underset{x \rightarrow 0}{\approx} \frac{1}{x}$$

$$\coth(x) \underset{|x| \rightarrow \infty}{\approx} \text{sign}(x)$$

we then can get for high temperatures ($K_B T \gg \frac{1}{2}\hbar\omega$):

$$\tilde{C}(\omega) = \frac{1}{\eta} \frac{2K_B T}{1 + (\omega\tau_\eta)^2}$$

and for the low temperatures ($K_B T \ll \frac{1}{2}\hbar\omega$):

$$\tilde{C}(\omega) = \frac{1}{\eta} \frac{\hbar|\omega|}{1 + (\omega\tau_\eta)^2}$$

The correlation function is the inverse Fourier Transform of $\tilde{C}(\omega)$.

a) For high temperatures we get:

$$C(\tau) = \int_{-\infty}^{+\infty} \frac{2K_B T}{\eta} \frac{d\omega}{2\pi} \frac{\exp[i\omega\tau]}{1 + (\omega\tau_\eta)^2}$$

and setting $\omega\tau_\eta = x$ we get the integral:

$$C(\tau) = \frac{K_B T}{\pi m} \int_{-\infty}^{\infty} \frac{\exp[ix\tau/\tau_\eta] dx}{1 + x^2}$$

using the residue theorem the integral is easily solvable:

$$C(\tau) = \frac{K_B T}{m} \exp\left[-\frac{\tau}{\tau_\eta}\right]$$

b) For low temperature the FT gives:

$$C(\tau) = -\frac{\hbar}{\pi\eta} \cdot \frac{1}{\tau^2}$$

5. since $T = 0$ we can take the low Temp. approximation in (4) and we have:

$$C_0 = \frac{\hbar}{\pi\eta}$$

6. Since the relations between the autocorrelation of v and x is (for $t = t_2 - t_1$):

$$C^{xx}(t) = \int_0^{t_2} \int_0^{t_1} \langle v(x)v(y) \rangle dx dy = \int_0^{t_2} \int_0^{t_1} \langle C^{vv}(x-y) \rangle dx dy$$

after some calculations we get:

$$\frac{d}{dt} S(t) = \int_0^t C(\tau) d\tau = \frac{\hbar}{\pi\eta} \frac{1}{t}$$

7. Using the result of (6) we get:

$$\int_{t_0}^t dS = \int_{t_0}^t \frac{dt}{t} \frac{\hbar}{\pi\eta}$$

and finally:

$$S(t) = S(t_0) + \frac{\hbar}{\pi\eta} \ln \left[\frac{t}{t_0} \right]$$