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hand in on 3th July 2015 before lecture

Advanced Statistical Physics II – Problem Sheet 11

Problem 1 – **Diffusion, velocity correlations and mean squared displacement**

Consider a freely diffusing particle in a viscous medium, governed by the Langevin equation,

$$m\dot{v}(t) = -\gamma v(t) + \delta F(t), \tag{1}$$

where m is the mass, γ is the friction constant, and $\delta F(t)$ is random forcing which fulfills $\langle \delta F(t) \rangle = 0$ and $\langle \delta F(t)\delta F(t')\rangle = 2\gamma k_B T \delta(t-t')$. The solution for the above equation is given as

$$v(t) = e^{-\gamma t/m}\left[v(0) + \int_0^t d\tau e^{\gamma\tau/m}\delta F(\tau)/m\right], \tag{2}$$

where $\langle v^2(0)\rangle = k_B T/m$.

a) i) By using Eq. (2) find the average position $\langle x(t)\rangle$.

ii) By using Eq. (2) calculate the mean squared displacement $\langle (x(t)-x(0))^2\rangle = \langle \int_0^t d\tau \int_0^t d\tau' v(\tau)v(\tau')\rangle$.

[*In Lecture the result has been shown and the derivation was partially shown. This time derive the result explicitly by showing the full calculation.*]

iii) By noting that the average position is $\langle x(t)\rangle$ and the variance is $\langle (x(t)-\langle x(t)\rangle)^2\rangle = \langle x^2(t)\rangle - \langle x(t)\rangle^2$, find the Gaussian probability distribution $\rho(x,t|x,0)$. Investigate two regimes $t \ll m/\gamma$ and $t \gg m/\gamma$, for $\rho(x,t|x,0)$. You will recover the well-known distribution for the position in the large t regime.

b) Now we use the Fourier transform $v(t) = \int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} v(\omega)/2\pi$ to find the velocity-velocity correlation $\langle v(t)v(t')\rangle$.

i) Find $v(\omega)$ from the Langevin equation Eq. (1) in Fourier space ω.

ii) Find $\langle v(\omega)v(\omega')\rangle$. For this calculate $\langle \delta F(\omega)\delta F(\omega')\rangle$.

iii) Find $\langle v(t)v(t')\rangle$ via the inverse Fourier transform. Use, if needed, $\int_0^\infty dx \cos(cx)/(a^2+b^2x^2) = \pi e^{-a|c|/b}/(2ab)$. Write down the autocorrelation function $\langle v(t)v(0)\rangle$ and $\langle v^2(t)\rangle$.

iv) By noting that the average velocity is $\langle v(t)\rangle = \langle v(0)\rangle\, e^{-\gamma t/m}$ and the variance is $\langle (v(t)-\langle v(t)\rangle)^2\rangle = \langle v^2(t)\rangle - \langle v(t)\rangle^2$, find the Gaussian probability distribution $\rho(v,t|v,0)$. Investigate two regimes $t \ll m/\gamma$ and $t \gg m/\gamma$, for $\rho(v,t|v,0)$. You will recover the well-known distribution for the velocity in the limit of $t \to \infty$.

Problem 2 – **Massive diffusing particle**

In the lecture we saw that for a massive particle in a harmonic trap, the Fourier transform of the response function is given by

$$\tilde{\chi}(\omega) = \frac{1}{-m\omega^2 - i\gamma\omega + k}. \tag{3}$$

a) Use the residue theorem to show that

$$\chi(t) \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} \tilde{\chi}(\omega)e^{-i\omega t}\, d\omega = \frac{\Theta(t)}{m\sqrt{k/m - \gamma^2/(4m^2)}} e^{-\gamma t/(2m)} \sin\left(\sqrt{\frac{k}{m} - \frac{\gamma^2}{4m^2}}\, t\right). \tag{4}$$

b) Calculate the response $x(t)$ to a force pulse at time zero (given by the force $F(t) = F_0\delta(t)$) and draw it schematically.

c) Consider now the special case of a free particle ($k \to 0$):

i) Show that in this case, equation (4) reduces to

$$\chi(t) = \frac{\Theta(t)}{\gamma}\left(1 - e^{-\gamma t/m}\right). \tag{5}$$

ii) Use the fluctuation-dissipation theorem to conclude that

$$C(t) - C(0) = -k_B T \int_0^t \chi(t')dt' = -\frac{k_\mathrm{B}T}{\gamma}\left[|t| + \frac{m}{\gamma}\left(e^{-\gamma|t|/m} - 1\right)\right], \tag{6}$$

where $C(t) = \langle x(t)x(0)\rangle$, and derive the limiting cases

$$C(t) - C(0) \approx \begin{cases} -k_\mathrm{B}T|t|^2/(2m) & t \ll m/\gamma \\ -k_\mathrm{B}T|t|/\gamma & t \gg m/\gamma. \end{cases} \tag{7}$$

d) Finally, take the zero-mass limit $m \to 0$ of equations (5), (6) to recover the result we derived for a freely diffusing massless particle in the lecture, i.e.

$$C(t) - C(0) = -\frac{k_\mathrm{B}T}{\gamma}|t|. \tag{8}$$