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Advanced Statistical Mechanics (WS 2019/20)
Problem Set 8

Problem 8: Diffusion in a quadratic potential

Here, we consider the relaxation of a diffusion process towards equilibrium:

$$\frac{\partial}{\partial t}P(x,t) = \frac{D}{2}\frac{\partial^2}{\partial x^2}P(x,t) - \frac{\partial}{\partial x}[v(x)P(x,t)] \tag{1}$$

with a deterministic velocity field $v(x) = -\Gamma \frac{d}{dx}U(x)$ and potential

$$U(x) = \frac{1}{2}x^2. \tag{2}$$

(a) Show that the equilibrium distribution is a Gaussian distribution

$$P_{\text{eq}}(x) = \frac{1}{\sqrt{2\pi\Delta_{\text{eq}}}}\exp\left[-\frac{1}{2\Delta_{\text{eq}}}(x-\mu_{\text{eq}})^2\right], \tag{3}$$

and calculate its mean μ_{eq} and variance Δ_{eq}.

(b) Let the initial distribution at time $t = 0$ be Gaussian with mean μ_0 and variance Δ_0. Show that the time-dependent solution $P_t(x) \equiv P(x,t)$ of the diffusion equation for $t > 0$ is also Gaussian and calculate the time-dependent mean $\mu(t)$ and variance $\Delta(t)$. Sketch the results for the following cases:

(i) $\mu_0 = \mu_{\text{eq}}, \Delta_0 \ll \Delta_{\text{eq}}$,
(ii) $\mu_0 = \mu_{\text{eq}}, \Delta_0 \gg \Delta_{\text{eq}}$,
(iii) $\mu_0 > \mu_{\text{eq}}, \Delta_0 = \Delta_{\text{eq}}$.

Hint: Assume that $P(x,t_1)$ at a given time t_1 is Gaussian distributed. Consider a small time-step δt and show that at time $t_2 = t_1 + \delta t$ the distribution $P(x,t_2)$ is in first order of δt of the form $A(t_1)\exp[B(x,t_1,t_2)]$, where $B(x,t_1,t_2)$ is quadratic in x. B can hence be written as $-(x-\mu(t_2))^2/2\Delta(t_2) + C(t_1,t_2)$. Express $\mu(t_2)$ and $\Delta(t_2)$ as functions of $\mu(t_1)$ and $\Delta(t_1)$. From that follow differential equations for $\mu(t)$ and $\Delta(t)$, which you have to solve. Check, if $P(x,t_2)$ is normalized properly.

(c) Calculate the Shannon entropy of time-dependent solution (minus its equilibrium value)

$$\mathcal{S}(t) - S_{\text{eq}} \equiv \mathcal{S}(P(t)) - \mathcal{S}(P_{\text{eq}}), \tag{4}$$

the expectation value of the energy (minus its equilibrium value)

$$\mathcal{U}(t) - \mathcal{U}_{\text{eq}} \equiv \int dx\, U(x)P(x,t) - \int dx\, U(x)P_{\text{eq}}(x), \tag{5}$$

and the resulting free entropy (minus its equilibrium value)

$$\Phi(t) - \Phi_{\text{eq}} \equiv (\mathcal{S}(t) - S_{\text{eq}}) - \beta(\mathcal{U}(t) - \mathcal{U}_{\text{eq}}) \tag{6}$$

with $\beta = 2\Gamma/D$. Discuss the behaviour for all three observables for the cases given in (b).

Remark: $1/\beta$ is the constant temperature of the reservoir, with which the system is in contact. In this diffusive problem the motion is over-damped, i.e. the kinetic energy is in equilibrium during the whole process and the dynamics only depend on the potential energy U.

To be discussed on: Mon, January 13th

Course information: `http://www.thp.uni-koeln.de/~lassig/teaching.html`