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Advanced Statistical Physics II – Problem Sheet 8

Problem 1 – **Stationary solution of the Fokker-Planck equation**

(2P) Show that the Boltzmann distribution $\rho_{\text{eq}}(x,p) \propto e^{-H(x,p)/k_BT}$ with $H(x,p) = U(p) + U(x)$ is a stationary solution of the Fokker-Planck equation for a massive particle in one dimension

$$\frac{\partial}{\partial t}\rho(x,p,t) = \left[-\frac{p}{m}\frac{\partial}{\partial x} + U'(x)\frac{\partial}{\partial p} + \frac{\gamma}{m}\frac{\partial}{\partial p}p + \gamma k_BT\frac{\partial^2}{\partial p^2}\right]\rho(x,p,t), \tag{1}$$

and find $U(p)$.

Problem 2 – **Mean first-passage time problems**

The mean first-passage time is the average time a particle needs to cross the barrier and reach x_B for the first time when starting at position $x_0 < x_B$. The formula for the mean first-passage time for the diffusivity D reads

$$\tau^{MFP} = \int_{x_0}^{x_B} \mathrm{d}x' \frac{\mathrm{e}^{\tilde{U}(x')}}{D} \int_{x_L}^{x'} \mathrm{d}x'' \mathrm{e}^{-\tilde{U}(x'')}, \tag{2}$$

where $x_L < x_0$ is the position of the reflective barrier and $\tilde{U} = U/k_BT$.

a) (1P) Consider a system confined in a box potential illustrated in figure 1 with infinitely high boundaries. Compute the mean first-passage time to reach x_B when starting at x_0.

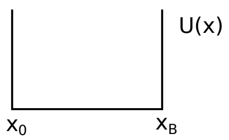

Figure 1

b) (3P) Consider the system illustrated in figure 2 and compute the mean first-passage time to reach x_B when starting at x_0. Discuss the limits $U_A \to \pm\infty$ and $x_L \to -\infty$.

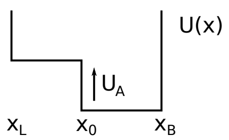

Figure 2

c) (4P) Now consider the simple multistate system illustrated in figure 3 and compute the mean first-passage time to reach x_B when starting at x_0. Explain te result and give an interpretation of the dominant term. Discuss the limits for $U_A \to \pm\infty$ and $U_B \to \pm\infty$.

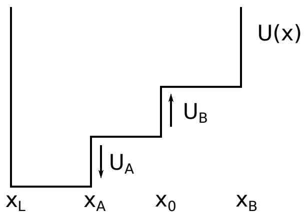

Figure 3

d) (3P) For the case $x_0 = x_L$, decompose the general expression (2) for the mean first passage time into three parts

$$\tau^{\text{MFP}} = \tau_I + \tau_{II} + \tau_R. \tag{3}$$

τ_I is the MFPT of a particle starting at $x_0 = x_L$ to reach the intermediate position x_1 with $x_0 < x_1 < x_B$. τ_{II} is the MFPT of a particle starting at x_1 to reach x_B without crossing x_1 again. How can τ_R be interpreted? Drawing paths helps.

Problem 3 – **Barrier-crossing problems**

a) (3P) Derive Kramers' formula for the barrier-crossing rate k

$$k = \frac{\sqrt{U''_A U''_B}}{2\pi\gamma} e^{-\Delta U / k_B T} \tag{4}$$

from the formula for the mean first-passage time given in problem 2 in eq. (2), using a saddlepoint approximation.

Hint: A saddlepoint approximation is a harmonic approximation at extremal points A, B of the potential $U(x)$ in the exponent and $U''_{A,B} = \left| \frac{\partial^2 U(x)}{\partial x^2} \right|_{A,B}$.

b) (1P) Guess how the Kramers' formula changes if the system can escape from the potential minimum in two directions in a one-dimensional landscape as illustrated in figure 4.

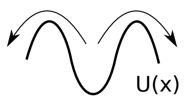

Figure 4

c) (3P) In biochemistry one often uses the empirical rule that at room temperature the reaction rate doubles when the temperature is increased by $10°$C. Compute the barrier height $\Delta U/k_BT$ for which this empirical rule follows from Arrhenius' law.