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T VI: Soft Matter and Biological Physics
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Problem set 2

Problem 2.1 *path integrals*
We shall show in this problem that the restricted partition sum

$$Z(x,t|x_0,0) \;=\; \int_{x(0)=x_0}^{x(t)=x} \mathcal{D}\left[x(\tau)\right] \exp\left(-\frac{1}{4D}\int_0^t \mathrm{d}\tau \left(\frac{\partial x}{\partial \tau}\right)^2 - \int_0^t \mathrm{d}\tau\, U\left(x\left(\tau\right)\right)\right)$$

obeys an equation of the Schrödinger type. First recall that the notation merely abbreviates a formal limit

$$Z(x,t|x_0,0) = \lim_{n\to\infty} \frac{1}{(4\pi D\epsilon)^{n/2}} \int \left[\prod_{k=1}^{n-1} \mathrm{d}x_k\right] \exp\left(-\frac{1}{4D\epsilon}\sum_{j=1}^{n-1}(x_{j+1}-x_j)^2 - \epsilon\sum_{j=1}^{n} U(x_j)\right), \qquad \epsilon = t/n\,,$$

with $x_n \equiv x$.

1. Then you may argue that the Chapman-Kolmogorov relation holds

   $$Z(x,t|x_0,0) = \int \mathrm{d}y\, Z(x,t|y,s)Z(y,s|x_0,0)\,.$$

   Do not try to be rigorous on the limiting procedure.

2. For small time differences Δt, the restricted partition sum $Z(x,t+\Delta t|y,t)$ is strongly peaked at $x \simeq y$, and one may approximate

   $$Z(x,t+\Delta t|y,t) \simeq \frac{1}{\sqrt{4D\Delta t}} \exp\left[-\frac{(x-y)^2}{4D\Delta t} - U(x)\Delta t\right]$$

   in leading order in Δt. Apply the Chapman-Kolmogorov relation for $t = s + \Delta t$ to show that

   $$\partial_t Z(x,t|x_0,0) = \left[D\nabla_x^2 - U(x)\right] Z(x,t|x_0,0)\,, \qquad Z(x,0|x_0,0) = \delta(x-x_0)\,.$$

Problem 2.2 *multiple integrals*
Demonstrate that the following relation holds

$$\left[\int_0^t f(\tau)\mathrm{d}\tau\right]^N = N! \int_0^t \mathrm{d}\tau_1 \int_0^{\tau_1} \mathrm{d}\tau_2 \ldots \int_0^{\tau_{N-1}} \mathrm{d}\tau_N f(\tau_1)\ldots f(\tau_N)\,.$$

Note that at the right hand side times are properly ordered $0 \le \tau_N \le \tau_{N-1} < \ldots < \tau_1 \le \tau_0 = 1$. It is helpful to show the property first for $N = 2$.

Problem 2.3 *diffusion*

A particle is diffusing in a region confined by hard walls, i.e. the probability density satisfies the diffusion equation

$$\partial_t \rho(x,t) = D\nabla_x^2 \rho(x,t)\,, \qquad -a/2 \leq x \leq a/2\,.$$

The walls are assumed to be reflecting which implies that the flux vanishes, $-D\nabla_x \rho(x = \pm a/2, t) = 0$. Solve the diffusion equation by expansion into appropriate eigenfunctions

$$\rho(x,t) = \sum_n \mathrm{e}^{-E_n t} c_n \varphi_n(x)\,.$$

Determine the solution for the initial condition $\rho(x, t = 0) = \delta(x - x_0)$. What does the density profile look like for long times?