Question 1. Classical systems and finite baths. Consider a Hamiltonian $H(q,p;\lambda)$ where (q,p) represents the generalized coordinates of a system of interest. The system is moved from one equilibrium state A into another equilibrium state B, as a control parameter λ varies from initial value λ_A to a final value λ_B, according to a driving protocol controlled by an external agent. In particular, the system is initially set in canonical equilibrium with temperature T at some value λ_A of the control parameter, and as it is driven, no energy is exchanged other than the work W performed by the agent.

a.) What are the assumptions we make to construct the time-reversed physical process, so that we can utilize finite bath formalism to explore this system?

b.) If one wants to calculate the work $W(q,p;t)$ done along this process for the specific phase trajectory that passes through the phase point (q,p) at time t, she considers precisely *one* such trajectory. Why?

c.) Write down $W(q,p;t)$ in terms of the Hamiltonian function (Hint: use a conservation law).

d.) Recall that the phase space density is conserved along any Hamiltonian trajectory, and write down $\rho(q,p,t)$ and $\tilde{\rho}(q,-p,t)$ in forward and backward process, respectively. Provide your answer in terms of partition functions Z_A (Z_B) of A (B).

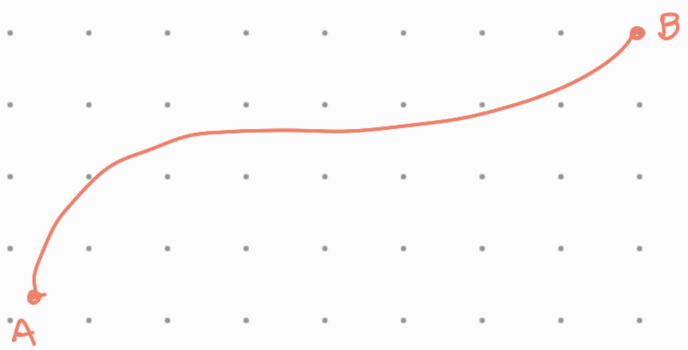
e.) Show that $\exp\{\beta[W(q,p;t)-\Delta F]\} = \frac{\rho(q,p,t)}{\tilde{\rho}(q,-p,t)}$.

f.) Use e.) and averaging methods of probability theory to prove $\langle W\rangle - \Delta F = kTD(\rho(q,p,t)\|\tilde{\rho}(q,-p,t))$.

g.) How do you interpret the expression in f.)? (Use verbal statements, provide physical intuition.)

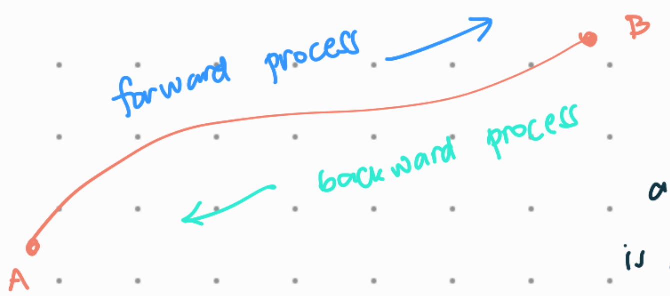
[12 marks: 1/1/2/2/2/2/2]

The system is moved from one equilibrium state A into another equilibrium state B, as a control parameter λ varies from initial value λ_A to a final value λ_B, according to a driving protocol controlled by an external agent.



a) The assumptions we make to construct the time-reversed physical process, so we can utilize finite bath formalism are:

(1)



the forward process due to control parameter $(\lambda(t))$ and the backward process is due to the same control parameter but reversed

② time-reversal symmetry of the Hamiltonian

$$\lambda(t) = \lambda(\tau - t)$$

b) To calculate the work $W(q, p; t)$ done along this process for the specific phase trajectory that passes through the phase point (q, p) at time t, there is precisely one such trajectory since the dynamics are deterministic. This is because the evolution of 1 state to another state is governed by Hamiltonian w/c is deterministic.

c) The $W(q, p; t)$ in terms of the Hamiltonian function is:

Using conservation law: Since no energy exchanged other than W, thus no heat in the system

$$\Delta E = Q + W$$

$$\Delta E = W$$

the change of energy is given by the difference of the Hamiltonian:

$$\Delta E = H(q_1, p_1; \lambda_B) - H(q_0, p_0; \lambda_A)$$

where:

q_0, p_0 = initial phase points $(t = 0)$

q_1, p_1 = final phase points $(t = \tau)$

thus:

$$W(q, p; t) = H(q_1, p_1; \lambda_B) - H(q_0, p_0; \lambda_A)$$

d) Phase space density is conserved along any Hamiltonian trajectory

↳ probability density (w/c follows a canonical distribution)

the forward process is:

$$\rho(q,p,t) = \rho(q_0, p_0, \underset{t_0=0}{t_0}) = \frac{e^{-\beta H(q_0, p_0; \lambda_A)}}{Z_A}$$

Z_A is the partition function

the backward process: now the system starts at initial condition $t = \tau$ w/ control parameter λ_B

$$\rho(q_1, -p_1, t) = \tilde{\rho}(q_1, -p, \underset{t_1=\tau}{t_1}) = \frac{e^{-\beta H(q_1, -p_1; \lambda_B)}}{Z_B}$$

this is $-p$ because:

for forward process: $p = mv = m\frac{dx}{dt}$

for backward process: $t' = \tau - t$

$dt' = -dt$

thus: $p = mv = -m\frac{dx}{dt}$

Z_B is the partition function

e) Show that $\exp\{\beta[W(q,p;t) - \Delta F\} = \dfrac{\rho(q,p,t)}{\tilde{\rho}(q,-p,t)}$

$$\frac{\rho(q,p,t)}{\tilde{\rho}(q,-p,t)} = \frac{\dfrac{e^{-\beta H(q_0, p_0; \lambda_A)}}{Z_A}}{\dfrac{e^{-\beta H(q_1, -p_1; \lambda_B)}}{Z_B}}$$

* H_B because the Hamiltonian is an even fn:
$H(q_1, -p_1; \lambda_B) = H(q_1, p_1; \lambda_B)$

$$= \frac{e^{-\beta \overbrace{H(q_0, p_0; \lambda_A)}^{H_A}}}{e^{-\beta \underbrace{H(q_1, -p_1; \lambda_B)}_{H_B^*}}} \cdot \frac{Z_B}{Z_A}$$

$$= e^{-\beta(H_A - H_B)} \cdot e^{\ln\left(\frac{Z_B}{Z_A}\right)}$$

$$= \exp\left(-\beta\,(\underbrace{H_A - H_B}_{-W(q,p;t)}) + \ln\left(\frac{Z_B}{Z_A}\right)\right)$$

since $\Delta F = -kT(\ln Z_B - \ln Z_A)$
free energy difference between the final and initial equilibrium

Finally, we have:
$$\exp(\beta W(q,p;t) - \Delta F) = \frac{\rho(q, p, t)}{\bar{\rho}(q, -p, t)}$$

f) use e to prove $\langle W \rangle - \Delta F = kT\, D(\rho(q,p,t) \,||\, \bar{\rho}(q,-p,t))$

$$\exp(\beta W(q,p;t) - \Delta F) = \frac{\rho(q, p, t)}{\bar{\rho}(q, -p, t)}$$

① take log of both sides:

$$\beta W(q,p;t) - \Delta F = \ln\left(\frac{\rho(q,p,t)}{\bar{\rho}(q,-p,t)}\right)$$

$$W(q,p,t) - \Delta F = k_B T \ln\left(\frac{\rho(q,p,t)}{\bar{\rho}(q,-p,t)}\right)$$

② multiply by ρ and take average

$$\int dq\,dp\,\rho W - \Delta F \underbrace{\int dq\,dp\,\rho}_{1} = k_B T \underbrace{\int dq\,dp\,\ln\frac{\rho(q,p,t)}{\bar{\rho}(q,-p,t)}}_{D(\rho(q,p,t)\,||\,\bar{\rho}(q,-p,t))}$$

$$\langle W \rangle - \Delta F = k_\beta T \, D(\rho(q, p, t) \,||\, \bar{\rho}(q, -p, t))$$

$$\langle W \rangle - \Delta F = k_\beta T \, D(\rho(q, p, t) \,||\, \bar{\rho}(q, -p, t))$$

g) The dissipated work $(\langle W \rangle - \Delta F)$ is revealed by the phase space density of forward and backward processes at any intermediate time of the experiment. And so when the forward and backward process is equal, then

$$\langle W \rangle - \Delta F = 0$$

since $D(\rho(q, p, t) \,||\, \rho(q, -p, t)) = 0$

which means that $\langle W \rangle = \Delta F$, thus no dissipated work

Question 2. Algorithmic complexity. Define the Kolmogorov algorithmic complexity K of a string of data. For a string of length N bits, how large might its Minimal Description Length be, and why? What relationship can be expected between the Kolmogorov complexity K and the Shannon entropy H given a set of data? [5 marks]

As discussed in the lecture awhile ago:

- the kolmogorov algorithmic complexity K of a string of data measures the complexity of a string s as the length of the shortest program that produces s

Formally, the Kolmogorov complexity is the minimal length of any string s: $C_u(s) = \min_p \{ L(p) : u(p) = s \}$
where we fix a UTM u, and defined $L(p)$ = length of string p

As an example:

$\underbrace{00 \ldots 0}_{10^5 \text{ times}}$ → small kolmogorov complexity (produced by a very short program)

While regular strings have small kolmogorov complexity, random strings have kolmogorov complexity approximately equal to their own length.

- From the Berry paradox, the minimal description length is N bits
- The relationship that can be expected between kolmogorov complexity K and the shannon entropy H is:

Expected algorithmic mutual information (from kolmogorov complexity) equals shannon mutual information:

$$I_p(X;Y) - K(p) \leq \sum_{x,y} P(x,y)\, I(x:y) \leq I_p(X;Y) + 2K(p)$$

From Shannon mutual information: $I_p(X;Y) = S(p(x)) - S(p(x|y))$
Algorithmic ——— : $I(x:y) = K(x) - K(x|y^*)$

Question 3. Stochastic thermodynamics and deterministic evolution. Consider a physical system X evolving under Hamiltonian dynamics. Let $\mathcal{T}_{t,0}(x \mid x_0)$ indicate the conditional probability that the system is in state x at time t, given initial state x_0 at time $t = 0$.

a.) Since X is governed by deterministic time evolution, conditional probability distribution $\mathcal{T}_{t,0}(x \mid x_0)$ should have the form of a Dirac-delta function. Can you write it down? [1 mark]

b.) Suppose you partition X into two subsystems, $X = A \times B$, and are only interested in the dynamics of subsystem A. Using some initial distribution $p(a, b)$, write down the conditional probability $\mathcal{T}_{t,0}(a \mid a_0)$ of finding A in state a at time t, given that it was initially in state a_0. [2 marks]

c.) In general, $\mathcal{T}_{t,0}(a \mid a_0)$ will be no longer deterministic. As we discussed many times in the lecture, if we marginalize out the subsystem B, subsystem A can evolve stochastically owing to statistical correlations with B. However, $\mathcal{T}_{t,0}(a \mid a_0)$ need not be Markovian in general (see the next component of this question). Supposing we have Markovian evolution over subsystem A, write down the form of the master equation for $0 < t' < t$, where LHS is $\mathcal{T}_{t,0}(a \mid a_0)$. [2 marks]

d.) To guarantee that the evolution of subsystem A is Markovian, we need two main assumptions. One of them concerns the initial probability distributions, and the other time scales. State the first one mathematically and the latter verbally. [2 marks]

e.) One of these two assumptions characterizes and / or justifies the definition of heat baths in stochastic thermodynamics. Which one? Can you explain how? [1 mark]

a) Let $T_{t,0}(x \mid x_0)$ indicate the conditional probability that system is in state x at time t, given initial state x_0 at time $t = 0$.

Since X is governed by deterministic time evolution, the conditional probability distribution $T_{t,0}(x \mid x_0)$ have this form:

$$T_{t,0}(x' \mid x) = \delta(x' - f(x_0))$$ where $f(x_0)$ trajectory of the Hamiltonian dynamics given initial state x_0

b) Suppose you partition X into 2 subsystems, $X = A \times B$, and are only interested in the dynamics of subsystem A. The conditional probability $T_{t,0}(a, a_0)$ of finding A in state a, at time t, given that it was initially at state a_0 is:

$$T_{t,0}(a, a_0) = \int \underbrace{T_{t,0}(a, b \mid a_0, b_0)}_{\text{prob. of being in } a,b \text{ given initial condition at } a_0, b_0} \underbrace{p_0(b_0 \mid a_0)}_{\text{prob. of being in } b_0, \text{ given initially at } a_0} \, db_0 \, db$$

c) The form of the master eqn for $0 < t' < t$, supposing we have a Markovian evolution over subsystem A is:

state a_0 at time $= 0$
a' at time $= t'$
a at time $= t$

$$T_{t,0}(a \mid a_0) = \int T_{t,t'}(a \mid a', a_0) \, T_{t',0}(a' \mid a_0) \, da'$$

Because we have a Markovian evolution

$$T_{t,0}(a \mid a_0) = \int T_{t,t'}(a \mid a') \, T_{t',0}(a' \mid a_0) \, da'$$

d) To guarantee that the evolution of subsystem A is Markovian, we need 2 assumptions: ① initial probability distribution

② timescales

① A and B are statistically independent at $t=0$
(sol is independent from bath)
$$P_0(a_0, b_0) = P_0(a_0)\, P_0(b_0)$$

② For condition 2, we assume that subsystem B instantly returns to some distribution B, w/c does not depend on the state of subsystem A. This leads to the separation of timescales, where subsystem B changes faster than subsystem A. That's why from subsystem A, it seems like B is in equilibrium.
This property characterizes subsystems w/c are called heat baths.

e) Condition 2 characterizes the definition of heat baths in Stochastic thermodynamics. Because of

separation of timescales - B relaxes instantly to P_t, since it is always in equilibrium.
(thus we can assume that temperature does not change)