1-1 Find the general solutions of the equations of motion

(A) $\begin{cases} \dot{r}(t) = \dfrac{p(t)}{m} \\ \dot{p}(t) = -\gamma\, p(t) \end{cases}$ (B) $\begin{cases} \dot{r}(t) = \dfrac{p(t)}{m} \\ \dot{p}(t) = -k\, r(t) \end{cases}$

Write down the corresponding changes of variables

$$(r, p) \xrightarrow{J_t} (r', p')$$

explicitly, and compute the corresponding Jacobians.

1-2 Take a system of one particle in $[0, L]$ 2

We consider two Hamiltonians $H_A(x,p) = \frac{p^2}{2m} + V(x)$

$H_B(x,p) = \frac{p^2}{2m}$

(a) Compute $\frac{Z_A(\beta)}{Z_B(\beta)}$

A→B Initially Hamiltonian is H_A and the system is in equilibrium at β. One then suddenly changes the Ham from H_A to H_B.

(b) What are possible valuse of the work W, and their probabilities?

(c) Compute $\langle e^{\beta \hat{W}_1} \rangle$ and $\langle \hat{W}_1 \rangle$

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$B \to A$ After a sufficiently long time, the distribution of the particle position x becomes uniform. (Why? Note that the system is isolated, and does not approach thermal equilibrium.)

One then suddenly changes the Ham from H_B to H_A.

(d) What are possible valuse of the work W_2 and their probabilities?

(e) Compute $\langle e^{\beta \hat{W}_2} \rangle$ and $\langle \hat{W}_2 \rangle$

(f) Compute $\langle e^{\beta(\hat{W}_1 + \hat{W}_2)} \rangle$ and $\langle \hat{W}_1 + \hat{W}_2 \rangle$

(g) Generalize the above results to the system of N non-interacting particles.

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1-3 We take the same setting as in p21, but do not assume time-reveral symmetry.
Prove that $\left\langle e^{-\Delta S_t(\hat{x})} \right\rangle_0 = 1$ and also show
$\langle \Delta S_t(\hat{x}) \rangle_0 \geq 0$ by using Jensen's inequality

1-4 Take the same setting as in "Fluctustion theorem" part.
By using p23-(3) show that

$$\langle \Delta S_t(\hat{x}) \rangle_0 = - \left\langle \Delta S_t(\hat{x})\, e^{-\Delta S_t(\hat{x})} \right\rangle_0$$

1-5 Confirm p25-(6)

2-1 Let $\hat{g}$ be a state quantity such that $g_j > 0$ for $\forall j$ 5

Show that $\prod_j (g_j^{p_j}) \leq \langle \hat{g} \rangle_{\mathbb{P}}$

(Note that this is a generalization of $\sqrt{ab} \leq \frac{a+b}{2}$ for $a, b > 0$)

2-2 Verify p15-(6)

2-3 Show that TT' is a stochastic matrix whe T and T' are stochastic matrices

see p.25

2-4 The stochastic matrix in P20-(1) is irreducible but not primitive if $\alpha = \beta = 1$. Examine which statements in Theorem of p.22 are valid or invalid

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2-5 Let T be a stochastic matrix. Assume that there is a probability distribution $\mathbb{P}^* = (P_j^*)_{j=1,\cdots,\Omega}$ such that

$T_{jk} P_k^* = T_{kj} P_j^*$ for any $k \neq j$

(we say that T satisfies the detailed balance condition with respect to $\mathbb{P}^*$)

Further assume T is primitive, and show that $\mathbb{P}^* = \mathbb{P}^S$

2-6 A stochstic matrix T is said to be doubly stochastic if $\sum_{k=1}^{\Omega} T_{jk} = 1$ for all j. Further assume that T is primitive, and show that $\mathbb{P}^S$ is the uniform distribution.

2-7 Take a quantum system with D-dim. Hilbert space, and let $\{|\varphi_j\rangle\}_{j=1,\cdots,D}$ and $\{|\psi_k\rangle\}_{k=1,\cdots,D}$ be orthonormal bases. For an arbitrary unitary operator $\hat{U}$, show that $T_{jk} = |\langle\varphi_j|\hat{U}|\psi_k\rangle|^2$ defines a doubly stochastic matrix T

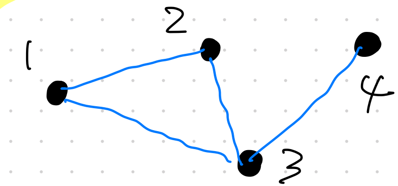
2-8 Consider an arbitrary graph (vertices connected by edges) whose vertices correspond to states $j = 1, \cdots, \Omega$. We write $j \sim k$ when the vertices (states) j and k are connected by an edge. We assume that the whole graph is connected.

define a stochastic matrix R by (lattice Laplacian)

$$R_{jk} = \begin{cases} 1 & \text{if } j \sim k \\ 0 & \text{if } j \neq k \text{ and } j \not\sim k \end{cases}$$

$$R_{jj} = -(\text{the number of } k \text{ s.t. } j \sim k)$$

example



$$R = \begin{pmatrix} -2 & 1 & 1 & 0 \\ 1 & -2 & 1 & 0 \\ 1 & 1 & -3 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}$$

Show that the uniform distribution $\mathbb{P}^S = \begin{pmatrix} 1/\Omega \\ \vdots \\ 1/\Omega \end{pmatrix}$ is the stationary distribution of the Markov jump process corresponding to general R

** 2-9 Let R be an irreducible transition rate matrix, and assume that there is a probability distribution $\mathbb{P}^* = (P_j^*)_{j=1,\cdots,\Omega}$ s.t. such that $R_{jk} P_k^* = R_{kj} P_j^*$ for any $j \neq k$.

(R satisfies the detailed balance condition with respect to $\mathbb{P}^*$)

Show that the general solution of the master equation $\dot{\mathbb{P}}(t) = R\,\mathbb{P}(t)$ is written as

$$\mathbb{P}(t) = \mathbb{P}^* + \sum_{l=2}^{\Omega} \alpha_l \, e^{\lambda_l t} v^{(l)}$$

with $\lambda_l < 0$ and vectors $v^{(l)}$ with real components. for $l = 2, \cdots, \Omega$

The real coefficients α_l are determined by the initial distribution $\mathbb{P}(0)$

(hint consider the matrix $\tilde{R} = (\tilde{R}_{jk})_{j,k=1,\cdots,\Omega}$ defined by $\tilde{R}_{jk} = \frac{1}{\sqrt{P_j^*}} R_{jk} \sqrt{P_k^*}$)

2-10 Let R be an irreducible transition rate matrix

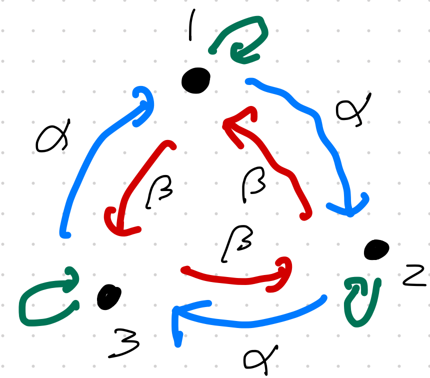
Prove that R satisfies the detailed balance condition with respect to some $\mathbb{P}^*$ if and only if

$$R_{j_1 j_2} R_{j_2 j_3} \cdots R_{j_n j_1} = R_{j_1 j_n} \cdots R_{j_3 j_2} R_{j_2 j_1} \quad (*)$$

for any $n = 3, \dots, \Omega$, and any $j_1, \dots, j_n$ s.t. $j_\ell \neq j_{\ell+1}$ and $j_1 \neq j_n$

2-11 Consider the Markov jump process with $\Omega = 3$

and the transition rate matrix defined by



$$R_{21} = R_{32} = R_{13} = \alpha$$

$$R_{12} = R_{23} = R_{31} = \beta$$

$$R_{11} = R_{22} = R_{33} = -(\alpha+\beta)$$

where $\alpha, \beta > 0$

Show that the process satisfies detailed balance condition only if $\alpha = \beta$

Find the general solution of the master equation $\dot{\mathbb{P}}(t) = R\,\mathbb{P}(t)$

2-12 Consider a Markov jump proces for $t \in [0, \tau]$ with the transition rates $\tilde{w}$ and the initial distribution $\mathbb{P}(0)$

Prove that

$$S(\mathbb{P}(\tau)) - S(\mathbb{P}(0)) + \langle\langle \hat{H}^{\tilde{w}} \rangle\rangle_{\mathbb{P}(0), \tilde{w}} \geq 0$$

the increase of the entropy of the system

the increase of the entropy of the heat bath

(total entropy production) ≥ 0

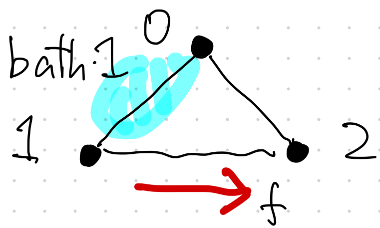
3-1 Verify the second equality in P9-(4)

☆ 3-2 Derive the Crooks fluctuation theorem, p12-(5)

☆☆ 3-3 Why does not the pump in p21 work?
(a qualitative explanation is sufficient)

4−1 We study the simplest possible model with $\Omega = 3$ that realizes the scenario in p.15.

states $j = 0, 1, 2$ $E_0 = -v,\ E_1 = E_2 = 0$



- bath 1 is coupled to the transitions $0 \longleftrightarrow 1$
- a non-conservative force f may act from 1 to 2

two jump quantities

$\hat{J}^{(A)}$ heat current to bath 1 $J^{(A)}_{0\to1} = -v,\ J^{(A)}_{1\to0} = v$

$J^{(A)}_{k\to j} = 0$ otherwise

$\hat{J}^{(B)}$ particle current from 1 to 2 $J^{(B)}_{1\to2} = 1,\ J^{(B)}_{2\to1} = -1$

$J^{(B)}_{k\to j} = 0$ otherwise

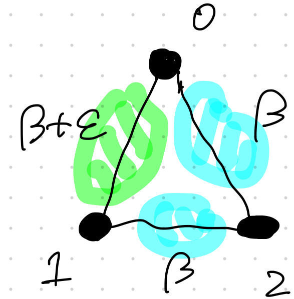
model A

no force, heat bath 1 has $\beta+\varepsilon$

$$w^{(A)}_{0\to1} = e^{-(\beta+\varepsilon)U}, \quad w^{(A)}_{1\to0} = 1$$

$$w^{(A)}_{0\to2} = e^{-\beta U}, \quad w^{(A)}_{2\to0} = 1$$

$$w^{(A)}_{1\to2} = w^{(A)}_{2\to1} = 1$$



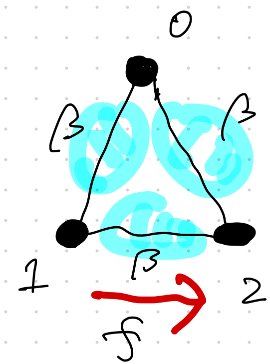
model B

heat bath 1 has β, force f from 1 to 2 ($\varepsilon = \beta f$)

$$w^{(B)}_{0\to1} = e^{-\beta U}, \quad w^{(B)}_{1\to0} = 1$$

$$w^{(B)}_{0\to2} = e^{-\beta U}, \quad w^{(B)}_{2\to0} = 1$$

$$w^{(B)}_{1\to2} = e^{\frac{\varepsilon}{2}}, \quad w^{(B)}_{2\to1} = e^{-\frac{\varepsilon}{2}}$$



Find the stationary distribution $\mathbb{P}^A$ for $\mathbb{W}^A$

Compute $\langle \hat{J}^{(B)} \rangle_{\mathbb{P}^A, \mathbb{W}^A}$ exactly and then expand it as

$$\langle \hat{J}^{(B)} \rangle_{\mathbb{P}^A, \mathbb{W}^A} = L_{BA}\, \varepsilon + O(\varepsilon^2)$$

Find the stationary distribution $\mathbb{P}^B$ for $\mathbb{W}^B$

Compute $\langle \hat{J}^{(A)} \rangle_{\mathbb{P}^B, \mathbb{W}^B}$ exactly and then expand it as

$$\langle \hat{J}^{(A)} \rangle_{\mathbb{P}^B, \mathbb{W}^B} = L_{AB}\, \varepsilon + O(\varepsilon^2)$$

Confirm that the reciprocal relation $L_{BA} = L_{AB}$ is valid