PHYSICS 210A : EQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #2 SOLUTIONS

(1) Consider a q-state generalization of the Kac ring model in which $\mathbb{Z}_q$ spins rotate around an N-site ring which contains a fraction $x = N_{\rm F}/N$ of flippers on its links. Each flipper cyclically rotates the spin values: $1 \to 2 \to 3 \to \cdots \to q \to 1$ (hence the clock model symmetry $\mathbb{Z}_q$).

(a) What is the Poincare recurrence time?

(b) Make the *Stosszahlansatz*, *i.e.* assume the spin flips are stochastic random processes. Then one has

$$P_\sigma(t+1) = (1-x)\,P_\sigma(t) + x\,P_{\sigma-1}(t)\ ,$$

where $P_0 \equiv P_q$. This defines a Markov chain

$$P_\sigma(t+1) = Q_{\sigma\sigma'}\,P_{\sigma'}(t)\ .$$

Decompose the transition matrix Q into its eigenvectors. *Hint:* The matrix may be diagonalized by a simple Fourier transform.

(c) The eigenvalues of Q may be written as $\lambda_\alpha = e^{-1/\tau_\alpha}\,e^{-i\delta_\alpha}$, where τ_α is a relaxation time and δ_α is a phase. Find the spectrum of relaxation times. What is the longest finite relaxation time?

(d) Suppose all the spins are initially in the state $\sigma = q$. Write down an expression for $P_\sigma(t)$ for all subsequent times $t \in \mathbb{Z}^+$. Plot your results for different values of x and q.

Solution:

(a) The recurrence time is $\tau = qN/\text{gcd}(N_{\rm F}, q)$, where $\text{gcd}(N_{\rm F}, q)$ is the greatest common divisor of $N_{\rm F}$ and q. After τ steps, which is to say $q/\text{gcd}(N_{\rm F}, q)$ cycles around the ring, each spin will have visited $qN_{\rm F}/\text{gcd}(N_{\rm F}, q)$ flippers. This is necessarily an integer multiple of q, which means that each spin will have mate $N_{\rm F}/\text{gcd}(N_{\rm F}, q)$ complete cycles of its internal $\mathbb{Z}_q$ clock.

(b) We have

$$Q_{\sigma\sigma'} = (1-x)\,\widetilde{\delta}_{\sigma,\sigma'} + x\,\widetilde{\delta}_{\sigma,\sigma'+1}\ ,$$

where

$$\widetilde{\delta}_{ij} = \begin{cases} 1 & \text{if } i = j \bmod q \\ 0 & \text{otherwise.} \end{cases}$$

Q is known as a *circulant matrix*, which is to say it satisfies $Q_{\sigma\sigma'} = Q(\sigma - \sigma' \bmod q)$. A circulant matrix of rank q has only q independent entries. Such a matrix may be brought to diagonal form by a unitary transformation: $Q = U\,\widehat{Q}\,U^\dagger$, where $U_{\sigma k} = \frac{1}{\sqrt{q}}\,e^{2\pi i k\sigma/q}$ and $\widehat{Q}_{kk'} \equiv \widehat{Q}(k)\,\widetilde{\delta}_{kk'}$ with

$$\widehat{Q}(k) = \sum_{n=1}^{q} Q(\mu)\,e^{-2\pi i k\mu/q}\ . \tag{1}$$

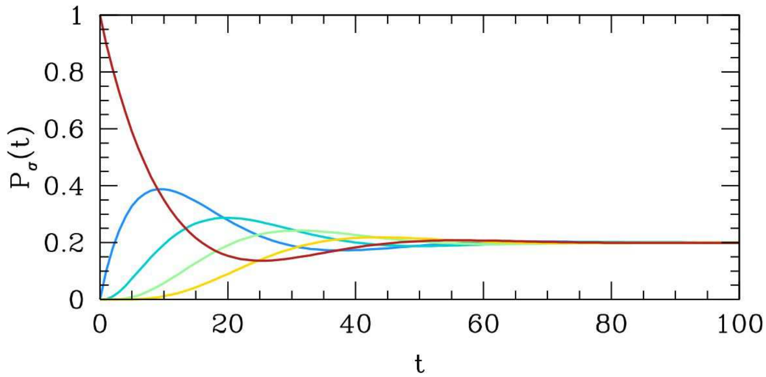

Figure 1: Behavior of $P_\sigma(t)$ for $q = 5$ and $x = 0.1$ within the *Stosszahlansatz* with initial conditions $P_\sigma(0) = \delta_{\sigma,q}$. Note that at large times the probabilities all converge to $\lim_{t\to\infty} P_\sigma(t) = q^{-1}$.

Since $Q(\mu) = (1-x)\,\widetilde{\delta}_{\mu,0} + x\,\widetilde{\delta}_{\mu,1}$, we have

$$\widehat{Q}(k) = 1 - x + x\,e^{-2\pi i k/q} \,.$$

(c) In the polar representation, we have $\widehat{Q}(k) = e^{-1/\tau_k(x)}\,e^{-i\delta_k(x)}$, where

$$\tau_k(x) = -\frac{2}{\ln\Big[1 - 2x(1-x)\big(1-\cos(2\pi k/q)\big)\Big]}$$

and

$$\delta_k(x) = \tan^{-1}\bigg(\frac{x\,\sin(2\pi k/q)}{1 - x + x\,\cos(2\pi k/q)}\bigg) \,.$$

Note that $\tau_q = \infty$, because the total probability is conserved by the Markov process. The longest finite relaxation time is $\tau_1 = \tau_{q-1}$.

(d) Given the initial conditions $P_\sigma(0) = \delta_{\sigma,q}$, we have

$$\begin{aligned} P_\sigma(t) &= (Q^t)_{\sigma\sigma'}\,P_{\sigma'}(0) \\ &= \frac{1}{q}\sum_{k=1}^{q} U_{\sigma k}\,\widehat{Q}^t(k)\,U^*_{\sigma' k}\,P_{\sigma'}(0) \\ &= \frac{1}{q}\sum_{k=1}^{q} e^{-t/\tau_k}\,e^{-it\delta_k}\,e^{2\pi i \sigma k/q} \,. \end{aligned}$$

We can combine the terms in the k sum by pairing k with $q-k$, since $\tau_{q-k} = \tau_k$ and $\delta_{q-k} = -\delta_k$. We should however consider separately the cases $k = q$ and, if q is even, $k = \frac{1}{2}q$, since for those values of k we have $\widehat{Q}(k)$ is real.

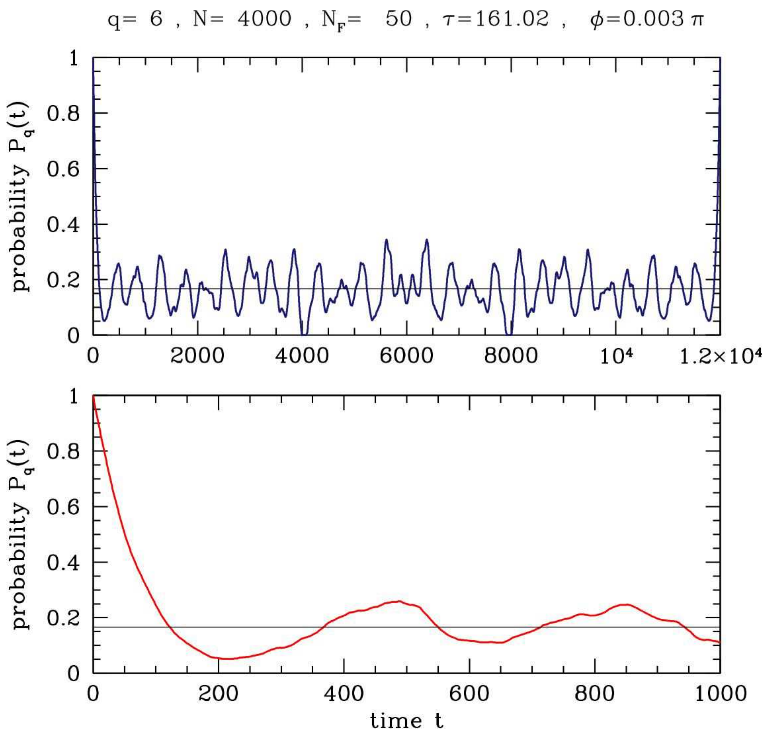

Figure 2: Evolution of the initial distribution $P_\sigma(0) = \delta_{\sigma,q}$ for the $\mathbb{Z}_q$ Kac ring model for $q = 6$, from a direct numerical simulation of the model.

If q is even, then $\widehat{Q}\big(k = \frac{1}{2}q\big) = 1 - 2x$. We then have

$$P_\sigma(t) = \frac{1}{q} + \frac{(-1)^\sigma}{q}\,(1-2x)^t + \frac{2}{q}\sum_{k=1}^{\frac{q}{2}-1} e^{-t/\tau_k(x)}\,\cos\!\left(\frac{2\pi\sigma k}{q} - t\,\delta_k(x)\right) .$$

If q is odd, then

$$P_\sigma(t) = \frac{1}{q} + \frac{2}{q}\sum_{k=1}^{\frac{q-1}{2}} e^{-t/\tau_k(x)}\,\cos\!\left(\frac{2\pi\sigma k}{q} - t\,\delta_k(x)\right) .$$

(e) See fig. 2.

(2) Consider a system with K possible states $|\,i\,\rangle$, with $i \in \{1,\ldots,K\}$, where the transition rate W_{ij} between any two states is the same, with $W_{ij} = \gamma > 0$.

(a) Find the matrix $\varGamma_{ij}$ governing the master equation $\dot{P}_i = -\varGamma_{ij}\,P_j$.

(b) Find all the eigenvalues and eigenvectors of $\varGamma$. What is the equilibrium distribution?

(c) Now suppose there are $2K$ possible states $|\,i\,\rangle$, with $i \in \{1,\ldots,2K\}$, and the transition rate matrix is

$$W_{ij} = \begin{cases} \alpha & \text{if} \quad (-1)^{ij} = +1 \\ \beta & \text{if} \quad (-1)^{ij} = -1 \ , \end{cases}$$

with $\alpha, \beta > 0$. Repeat parts (a) and (b) for this system.

Solution :

(a) We have

$$\Gamma_{ij} = \begin{cases} -W_{ij} = -\gamma & \text{if } i \neq j \\ \sum_k' W_{kj} = (K-1)\gamma & \text{if } i = j \ . \end{cases}$$

I.e. Γ is a symmetric $K \times K$ matrix with all off-diagonal entries $-\gamma$ and all diagonal entries $(K-1)\gamma$.

(b) It is convenient to define the unit vector $\boldsymbol{\psi} = K^{-1/2}(1, 1, \ldots, 1)$. Then

$$\Gamma = K\gamma \left(\mathbb{I} - |\,\psi\,\rangle\langle\,\psi\,| \right) .$$

We now see that $|\,\psi\,\rangle$ is an eigenvector of Γ with eigenvalue $\lambda = 0$, and furthermore that any vector orthogonal to $|\,\psi\,\rangle$ is an eigenvector of Γ with eigenvalue $K\gamma$. This means that there is a degenerate $(K-1)$-dimensional subspace associated with the eigenvalue $K\gamma$. The equilibrium distribution is given by $|\,P^{\text{eq}}\,\rangle = K^{-1/2}|\,\psi\,\rangle$, *i.e.* $P_i^{\text{eq}} = K^{-1}$.

(c) Define the unit vectors

$$\begin{aligned} \boldsymbol{\psi}_{\mathsf{e}} &= \tfrac{1}{\sqrt{K}} \left(0, 1, 0, \ldots, 1\right) \\ \boldsymbol{\psi}_{\mathsf{o}} &= \tfrac{1}{\sqrt{K}} \left(1, 0, 1, \ldots, 0\right) . \end{aligned}$$

Note that $\langle\,\psi_{\mathsf{e}}\,|\,\psi_{\mathsf{o}}\,\rangle = 0$. Furthermore, we may write Γ as

$$\Gamma = \tfrac{1}{2}K(3\alpha+\beta)\,\mathbb{I} + \tfrac{1}{2}K(\alpha-\beta)\,\mathbb{J} - K\alpha \left(|\,\psi_{\mathsf{e}}\,\rangle\langle\,\psi_{\mathsf{e}}\,| + |\,\psi_{\mathsf{o}}\,\rangle\langle\,\psi_{\mathsf{e}}\,| + |\,\psi_{\mathsf{e}}\,\rangle\langle\,\psi_{\mathsf{o}}\,| \right) - K\beta\,|\,\psi_{\mathsf{o}}\,\rangle\langle\,\psi_{\mathsf{o}}\,|$$

where $\mathbb{I}$ is the identity matrix and $\mathbb{J}_{nn'} = (-1)^n\,\delta_{nn'}$ is a diagonal matrix with alternating -1 and $+1$ entries. Note that $\mathbb{J}\,|\,\psi_{\mathsf{o}}\,\rangle = -|\,\psi_{\mathsf{o}}\,\rangle$ and $\mathbb{J}\,|\,\psi_{\mathsf{e}}\,\rangle = +|\,\psi_{\mathsf{e}}\,\rangle$. The key to deriving the above relation is to notice that

$$\begin{aligned} \mathbb{M} &= K\alpha \left(|\,\psi_{\mathsf{e}}\,\rangle\langle\,\psi_{\mathsf{e}}\,| + |\,\psi_{\mathsf{o}}\,\rangle\langle\,\psi_{\mathsf{e}}\,| + |\,\psi_{\mathsf{e}}\,\rangle\langle\,\psi_{\mathsf{o}}\,| \right) + K\beta\,|\,\psi_{\mathsf{o}}\,\rangle\langle\,\psi_{\mathsf{o}}\,| \\ &= \begin{pmatrix} \beta & \alpha & \beta & \alpha & \cdots & \beta & \alpha \\ \alpha & \alpha & \alpha & \alpha & \cdots & \alpha & \alpha \\ \beta & \alpha & \beta & \alpha & \cdots & \beta & \alpha \\ \alpha & \alpha & \alpha & \alpha & \cdots & \alpha & \alpha \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \beta & \alpha & \beta & \alpha & \cdots & \beta & \alpha \\ \alpha & \alpha & \alpha & \alpha & \cdots & \alpha & \alpha \end{pmatrix} . \end{aligned}$$

Now $\mathbb{J}$ has K eigenvalues $+1$ and K eigenvalues -1. There is therefore a $(K-1)$-dimensional degenerate eigenspace of Γ with eigenvalue $2K\alpha$ and a $(K-1)$-dimensional degenerate subspace with eigenvalue $K(\alpha+\beta)$. These subspaces are mutually orthogonal as well as being orthogonal to the vectors $|\,\psi_{\mathsf{e}}\,\rangle$ and $|\,\psi_{\mathsf{o}}\,\rangle$. The remaining two-dimensional subspace spanned by these vectors yields the reduced matrix

$$\Gamma_{\rm red} = \begin{pmatrix} \langle\,\psi_{\mathsf{e}}\,|\,\Gamma\,|\,\psi_{\mathsf{e}}\,\rangle & \langle\,\psi_{\mathsf{e}}\,|\,\Gamma\,|\,\psi_{\mathsf{o}}\,\rangle \\ \langle\,\psi_{\mathsf{o}}\,|\,\Gamma\,|\,\psi_{\mathsf{e}}\,\rangle & \langle\,\psi_{\mathsf{o}}\,|\,\Gamma\,|\,\psi_{\mathsf{o}}\,\rangle \end{pmatrix} = \begin{pmatrix} K\alpha & -K\alpha \\ -K\alpha & K\alpha \end{pmatrix} .$$

The eigenvalues in this subspace are therefore 0 and $2K\alpha$. Thus, Γ has the following eigenvalues:

$$\begin{aligned} &\lambda = 0 && \text{(nondegenerate)} \\ &\lambda = K(\alpha+\beta) && \text{(degeneracy } K-1) \\ &\lambda = 2K\alpha && \text{(degeneracy } K) . \end{aligned}$$

(3) A generalized two-dimensional cat map can be defined by

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \overbrace{\begin{pmatrix} 1 & p \\ q & pq+1 \end{pmatrix}}^{M} \begin{pmatrix} x \\ y \end{pmatrix} \ \text{mod}\ \mathbb{Z}^2 ,$$

where p and q are integers. Here $x, y \in [0,1]$ are two real numbers on the unit interval, so $(x,y) \in \mathbb{T}^2$ lives on a two-dimensional torus. The inverse map is

$$M^{-1} = \begin{pmatrix} pq+1 & -p \\ -q & q \end{pmatrix} .$$

Note that det $M = 1$.

(a) Consider the action of this map on a pixelated image of size $(lK)\times(lK)$, where $l \sim 4-10$ and $K \sim 20-100$. Starting with an initial state in which all the pixels in the left half of the array are "on" and the others are all "off", iterate the image with the generalized cat map, and compute at each state the entropy $S = -\sum_{\boldsymbol{r}} p_{\boldsymbol{r}} \log_2 p_{\boldsymbol{r}}$, where the sum is over the K^2 different $l \times l$ subblocks, and $p_{\boldsymbol{r}}$ is the probability to find an "on" pixel in subblock $\boldsymbol{r}$. (Take $p = q = 1$ for convenience, though you might want to explore other values.)

Now consider a three-dimensional generalization (Chen *et al.*, *Chaos, Solitons, and Fractals* **21**, 749 (2004)), with

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = M \begin{pmatrix} x \\ y \\ z \end{pmatrix} \ \text{mod}\ \mathbb{Z}^3 ,$$

which is a discrete automorphism of $\mathbb{T}^3$, the three-dimensional torus. Again, we require that both M and M^{-1} have integer coefficients. This can be guaranteed by writing

$$M_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & p_x \\ 0 & q_x & p_x q_x + 1 \end{pmatrix} \quad , \quad M_y = \begin{pmatrix} 1 & 0 & p_y \\ 0 & 1 & 0 \\ q_y & 0 & p_y q_y + 1 \end{pmatrix} \quad , \quad M_z = \begin{pmatrix} 1 & p_z & 0 \\ q_z & p_z q_z + 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and taking $M = M_x M_y M_z$, reminiscent of how we build a general $\mathsf{O}(3)$ rotation from a product of three $\mathsf{O}(2)$ rotations about different axes.

(b) Find M and M^{-1} when $p_x = q_x = p_y = q_y = p_z = q_z = 1$.

(c) Repeat part (a) for this three-dimensional generalized cat map, computing the entropy by summing over the K^3 different $l \times l \times l$ subblocks.

(d) 100 quatloos extra credit if you find a way to show how a three dimensional object (a ball, say) evolves under this map. Is it Poincaré recurrent?

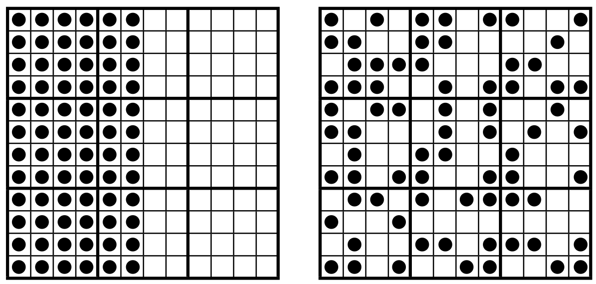

Figure 3: Two-dimensional cat map on a 12×12 square array with $l = 4$ and $K = 3$ shown. Left: initial conditions at $t = 0$. Right: possible conditions at some later time $t > 0$. Within each $l \times l$ cell $\boldsymbol{r}$, the occupation probability $p_{\boldsymbol{r}}$ is computed. The entropy $-p_{\boldsymbol{r}} \log_2 p_{\boldsymbol{r}}$ is then averaged over the K^2 cells.

Solution :

(a) See figs. 4 and 5.

(b) We have

$$M_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 2 \end{pmatrix} \quad , \quad M_y = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 2 \end{pmatrix} \quad , \quad M_z = \begin{pmatrix} 1 & 1 & 0 \\ 1 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and

$$M_x^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & -1 \\ 0 & -1 & 1 \end{pmatrix} \quad , \quad M_y^{-1} = \begin{pmatrix} 2 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad , \quad M_z^{-1} = \begin{pmatrix} 2 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad .$$

Thus,

$$M = M_x M_y M_z = \begin{pmatrix} 1 & 1 & 1 \\ 2 & 3 & 2 \\ 3 & 4 & 4 \end{pmatrix}$$

and

$$M^{-1} = M_z^{-1} M_y^{-1} M_x^{-1} = \begin{pmatrix} 4 & 0 & -1 \\ -2 & 1 & 0 \\ -1 & -1 & 1 \end{pmatrix} \ .$$

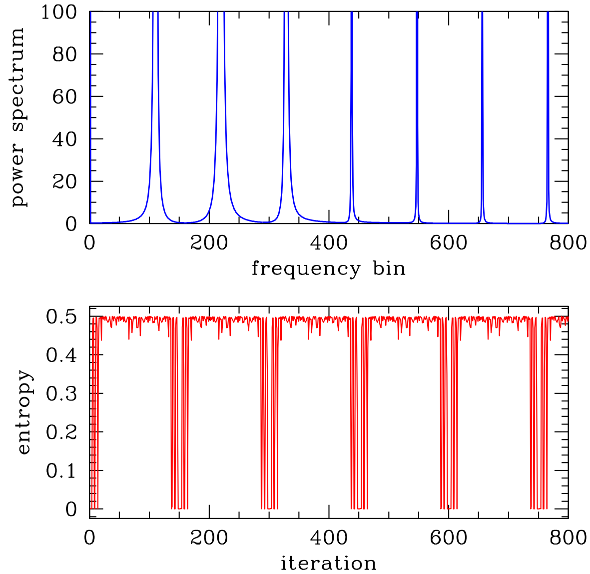

Figure 4: Coarse-grained entropy per unit volume for the iterated two-dimensional cat map ($p = q = 1$) on a 200×200 pixelated torus, with $l = 4$ and $K = 50$. Bottom panel: coarse-grained entropy per unit volume *versus* iteration number. Top panel: power spectrum of entropy *versus* frequency bin. A total of $2^{14} = 16384$ iterations were used.

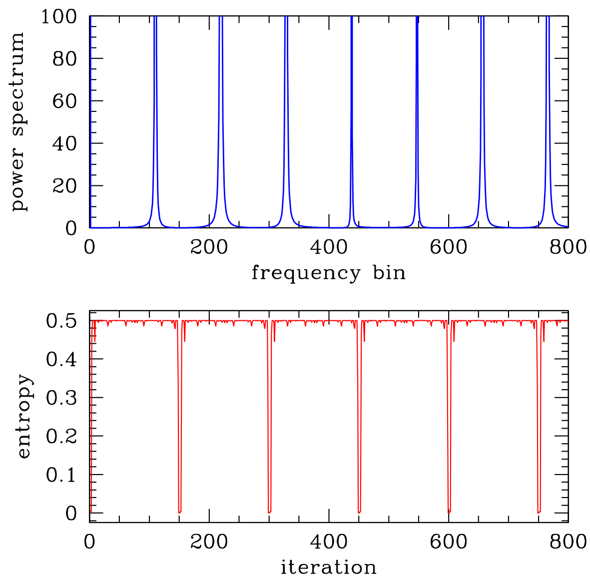

Figure 5: Same as in fig. 4 but with $l = 10$ and $K = 20$.

Note that $\det M = 1$.

(c) See fig. 6.

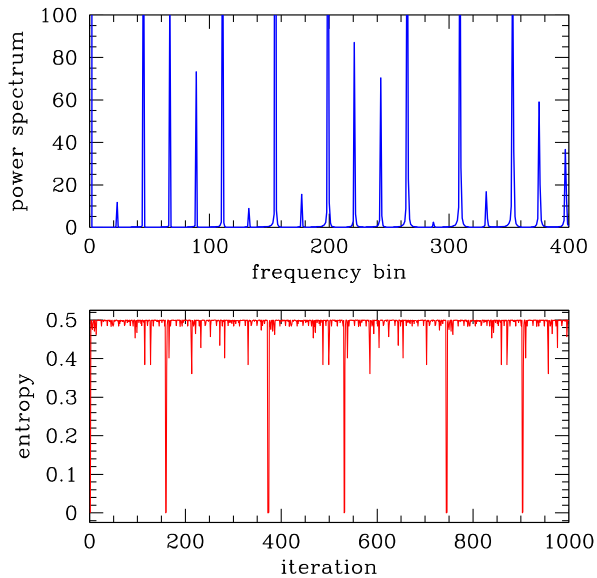

Figure 6: Coarse-grained entropy per unit volume for the iterated three-dimensional cat map ($p_x = q_x = p_y = q_y = p_z = q_z = 1$) on a $40 \times 40 \times 40$ pixelated three-dimensional torus, with $l = 4$ and $K = 10$. Bottom panel: coarse-grained entropy per unit volume *versus* iteration number. Top panel: power spectrum of entropy *versus* frequency bin. A total of $2^{14} = 16384$ iterations were used.

(d) On a $k \times k \times k$ grid, there are 2^{k^3} possible pixelated images. The $3d$ cat map then uniquely and reversibly maps between different elements of this set. Thus the map is recurrent.

(4) Consider a d-dimensional ideal gas with dispersion $\varepsilon(\boldsymbol{p}) = A|\boldsymbol{p}|^\alpha$, with $\alpha > 0$. Find the density of states $D(E, V, N)$, the statistical entropy $S(E, V, N)$, the equation of state $p = p(T, V, N)$, the heat capacity at constant volume $C_{V,N}(T, V, N)$, and the heat capacity at constant pressure $C_{p,N}(T, V, N)$. (Particle number N is held constant.) Recall the thermodynamic relation

$$dS = \frac{1}{T}\,dE + \frac{p}{T}\,dV - \frac{\mu}{T}\,dN \quad ,$$

Solution :

The density of states is

$$D(E, V, N) = \frac{V^N}{N!} \int \frac{d^d p_1}{h^d} \cdots \int \frac{d^d p_N}{h^d}\, \delta\big(E - Ap_1^\alpha - \ldots - Ap_N^\alpha\big)\,.$$

The Laplace transform is

$$\begin{aligned}
\widehat{D}(\beta,V,N) &= \frac{V^N}{N!}\bigg(\int\!\frac{d^d\!p}{h^d}\,e^{-\beta A p^\alpha}\bigg)^N \\
&= \frac{V^N}{N!}\bigg(\frac{\Omega_d}{h^d}\int\limits_0^\infty\!\!dp\,p^{d-1}\,e^{-\beta A p^\alpha}\bigg)^N \\
&= \frac{V^N}{N!}\bigg(\frac{\Omega_d\,\Gamma(d/\alpha)}{\alpha h^d A^{d/\alpha}}\bigg)^N \beta^{-Nd/\alpha}\ .
\end{aligned}$$

Now we inverse transform, recalling

$$K(E)=\frac{E^{t-1}}{\Gamma(t)} \qquad \Longleftrightarrow \qquad \widehat{K}(\beta)=\beta^{-t}\ .$$

We then conclude

$$D(E,V,N)=\frac{V^N}{N!}\bigg(\frac{\Omega_d\,\Gamma(d/\alpha)}{\alpha h^d A^{d/\alpha}}\bigg)^N \frac{E^{\frac{Nd}{\alpha}-1}}{\Gamma(Nd/\alpha)}$$

and

$$\begin{aligned}
S(E,V,N) &= k_{\rm B}\ln D(E,V,N) \\
&= Nk_{\rm B}\ln\!\bigg(\frac{V}{N}\bigg)+\frac{d}{\alpha}\,Nk_{\rm B}\,\ln\!\bigg(\frac{E}{N}\bigg)+Na_0\ ,
\end{aligned}$$

where a_0 is a constant, and we take the thermodynamic limit $N\to\infty$ with V/N and E/N fixed. From this we obtain the differential relation

$$\begin{aligned}
dS &= \frac{Nk_{\rm B}}{V}\,dV+\frac{d}{\alpha}\,\frac{Nk_{\rm B}}{E}\,dE+s_0\,dN \\
&= \frac{p}{T}\,dV+\frac{1}{T}\,dE-\frac{\mu}{T}\,dN\ ,
\end{aligned}$$

where s_0 is a constant. From the coefficients of dV and dE, we conclude

$$\begin{aligned}
pV &= Nk_{\rm B}T \\
E &= \frac{d}{\alpha}\,Nk_{\rm B}T\ .
\end{aligned}$$

Setting $dN=0$, we have

$$\begin{aligned}
đQ &= dE+p\,dV \\
&= \frac{d}{\alpha}\,Nk_{\rm B}\,dT+p\,dV \\
&= \frac{d}{\alpha}\,Nk_{\rm B}\,dT+p\,d\bigg(\frac{Nk_{\rm B}T}{p}\bigg)\ .
\end{aligned}$$

Thus,

$$C_{V,N}=\frac{đQ}{dT}\bigg|_{V,N}=\frac{d}{\alpha}\,Nk_{\rm B} \quad , \quad C_{p,N}=\frac{đQ}{dT}\bigg|_{p,N}=\bigg(1+\frac{d}{\alpha}\bigg)Nk_{\rm B}\ .$$

(5) Write a well-defined expression for the greatest possible number expressible using only five symbols. *Examples:* $1+2+3$, 10^{100}, $\Gamma(99)$. `[50 quatloos extra credit]`

Solution :

Using conventional notation, my best shot would be $9^{9^{9^{9^{9}}}}$. This is a very big number indeed: $9^9 \approx 3.73 \times 10^8$, so $9^{9^9} \sim 10^{3.7\times 10^8}$, and $9^{9^{9^{9}}} \sim 10^{10^{10^{3.7\times 10^8}}}$. But in the world of big numbers, this is still tiny. For a fun diversion, use teh google to learn about the Ackermann sequence and Knuth's up-arrow notation. Using Knuth's notation, described in

`https://en.wikipedia.org/wiki/Knuth%27s_up-arrow_notation` ,

one could write $9 \uparrow^{99} 9$, which is vastly larger than the puny $9^{9^{9^{9^{9}}}}$. But even *these* numbers are modest compared with something called the "Busy Beaver sequence", which is a concept from computer science and Turing machines. For a very engaging essay on large numbers, see `https://www.scottaaronson.com/blog/?p=3445`.