

STATISTICAL MECHANICS OF COMPLEX SYSTEMS – SOLUTIONS 2010

1. (a) All entropy formulae below have an arbitrary multiplicative constant K setting the units, or alternatively an arbitrary base of the logarithm.

joint information entropy:

$$H(X, Y) = - \sum_{i,j} p_{ij} \log p_{ij} \quad \{2\}$$

conditional information entropies:

$$H(X|Y) = \sum_j p_j^{(Y)} H(X|Y = y_j) = - \sum_{i,j} p_{ij} \log \frac{p_{ij}}{p_j^{(Y)}} \quad \{2\}$$

$$H(Y|X) = \sum_i p_i^{(X)} H(Y|X = x_i) = - \sum_{i,j} p_{ij} \log \frac{p_{ij}}{p_i^{(X)}} \quad \{2\}$$

mutual information:

$$I(X; Y) = \sum_{i,j} p_{ij} \log \frac{p_{ij}}{p_i^{(X)} p_j^{(Y)}} \quad \{2\}$$

[Bookwork]

- (b) Three independent relations:

$$H(X|Y) = H(X, Y) - H(Y)$$

$$H(Y|X) = H(X, Y) - H(X)$$

$$I(X; Y) = H(X) + H(Y) - H(X, Y)$$

any set of independent relations worth $\{2\}$ per equation.

[Bookwork]

- (c) Using notation $\{e, o\}$ for even, odd (for V) and $\{p, n\}$ for prime, non-prime (for W), the joint probabilities: $p_{ep} = 1/6$, $p_{en} = 1/3$, $p_{op} = 1/3$, $p_{on} = 1/6$. Using bits as units (using \log_2), the joint entropy:

$$H(V, W) = - \left(\frac{1}{6} \log_2 \frac{1}{6} + \frac{1}{3} \log_2 \frac{1}{3} + \frac{1}{3} \log_2 \frac{1}{3} + \frac{1}{6} \log_2 \frac{1}{6} \right) \quad \{1\}$$

$$= \frac{1}{3} \log_2 6 + \frac{2}{3} \log_2 3 = \log_2 3 + \frac{1}{3} \quad \{1\}$$

$$= \frac{\ln 3}{\ln 2} + \frac{1}{3} \approx 1.92 \text{ bit}$$

One way to calculate the mutual information is to realise that $p_e = p_o = 1/2$, so $H(V) = -2 \frac{1}{2} \log_2 \frac{1}{2} = 1$ bit, similarly $H(W) = 1$ bit. $\{1\}$

Then

$$\begin{aligned} I(V; W) &= H(V) + H(W) - H(V, W) \\ &= 1 + 1 - \left(\log_2 3 + \frac{1}{3} \right) = \frac{5}{3} - \log_2 3 \quad \{2\} \\ &\approx 0.08 \text{ bit} \end{aligned}$$

Alternatively, one can apply the formula in 1(a).

[Unseen]

- (d) (i) False. They don't even have the same units (eg. bit vs bit²) ! {2}
A numerical counterexample (using bits as units): if X and Y are independent coin tosses, $H(X) = H(Y) = 1$, $H(X, Y) = 2 \neq 1 \cdot 1$.
- (ii) False. It can be easily shown that $H(X, X) = H(X)$ (eg. by applying the definition). Then $H(X|X) = H(X, X) - H(X) = 0$, so any nontrivial X is counterexample. {2}
- (iii) True. $I(X; X) = H(X) + H(X) - H(X, X) = H(X)$. {2}
- [Unseen]**

2. (a) Interface width:

$$w(L, t) = \sqrt{\langle (h(x, t) - \bar{h}(t))^2 \rangle_x} \quad \text{where} \quad \bar{h}(t) = \langle h(x, t) \rangle_x \quad \{1\}$$

[Bookwork]

- (b) (i) early times, $t \ll t_\times$: $w(L, t) \sim t^\beta$ β : growth exponent $\{2\}$
 late times, $t \gg t_\times$: $w(L, t) \sim w_{\text{sat}}(L) \sim L^\alpha$ α : roughness exponent $\{2\}$
 crossover time: $t_\times \sim L^z$ z : dynamic exponent $\{2\}$

[Bookwork]

(ii) Family-Vicsek scaling relation:

$$w(L, t) \sim L^\alpha f\left(\frac{t}{L^z}\right) \quad f(u) \sim \begin{cases} u^\beta, & \text{if } u \ll 1 \\ \text{const}, & \text{if } u \gg 1 \end{cases} \quad \{2\}$$

For $t \ll L^z$: $W(L, t) \sim L^\alpha \cdot (t/L^z)^\beta \sim t^\beta$ (using $z = \alpha/\beta$)

For $t \gg L^z$: $W(L, t) \sim L^\alpha \cdot \text{const} \sim L^\alpha$. $\{1\}$

[Bookwork]

(iii) To recover t^β for small t , we need $g(u) = \text{const}$ for $u \gg 1$ (assuming $B > 0$) to make it independent of L , which sets $A = \beta$. $\{1\}$

To obtain L^α for large t , we need $g(u) = u^\alpha$ for $u \ll 1$. $\{2\}$

Then for large t , $L^\alpha \sim w \sim t^\beta L^\alpha t^{-B\alpha}$. This gives $B = \beta/\alpha = 1/z$. $\{2\}$

In summary:

$$w(L, t) \sim t^\beta g\left(\frac{L}{t^{1/z}}\right) \quad g(u) \sim \begin{cases} u^\alpha, & \text{if } u \ll 1 \\ \text{const}, & \text{if } u \gg 1 \end{cases}$$

[Unseen]

(c) (i) Random deposition model: the interface grows on a discretised substrate by accreting squares (hypercubes in general dimension). The cubes arrive above random substrate positions, and simply increase the height of the column at that position.

[Bookwork] $\{2\}$

(ii) Suppose N cubes are grown on a substrate made of S units. (In one dimension $S = L$, in two dimensions $S = L^2$ etc.) The growth above a given substrate location can be considered as the sum of N i.i.d Bernoulli processes, each grows unit height ($\Delta h = 1$) with probability $p = 1/S$ and does not grow ($\Delta h = 0$) with probability $1 - p$. The expectation $\langle \Delta h \rangle = p = 1/S$, and the variance $\text{Var}(\Delta h) = \langle (\Delta h)^2 \rangle - \langle \Delta h \rangle^2 = p(1 - p) = (S - 1)/S^2$, since $\langle (\Delta h)^2 \rangle = p$ $\{3\}$

The Central Limit Theorem says that the sum of N such processes has mean $\bar{h} = N\langle \Delta h \rangle = N/S$, and variance

$$\langle (h - \bar{h})^2 \rangle = N\text{Var}(\Delta h) = N \frac{S - 1}{S^2} = w^2 \quad \{2\}$$

which equals to the square of the interface width. Now fix the substrate size S . If time is measured as N (maybe with some proportionality constant, eg. $t = N/S$; this does not change the scaling exponent), then

$$w \sim \sqrt{N} \sim \sqrt{t}$$

using $w \sim t^\beta$, this gives $\beta = 1/2$. $\{1\}$

[Unseen]

(iii)

$$\frac{\partial h}{\partial t} = F + \eta(x, t)$$

Where η has zero mean and is delta correlated:

$$\langle \eta(x, t) \rangle = 0$$

$$\langle \eta(x, t) \eta(x', t') \rangle = 2D \delta(x - x') \delta(t - t')$$

{2}

[Bookwork]

3. (a) The laws of thermodynamics (credit {1} for each):
- (0) There exist a relation between thermodynamic systems. This relation is called thermodynamic equilibrium, and it is transitive (equivalence relation):
if $A \sim B$ and $B \sim C$, then $A \sim C$.
Here A , B and C label different systems. For example in thermal equilibrium this means a transitive relation between the temperatures of the three systems.
 - (1) Energy conservation: the total energy of an isolated system is fixed.
Thus if during some process a system absorbs heat ΔQ , as well as work $\Delta W = -p \Delta V + \dots$ is made on it, then its energy changes by $\Delta E = \Delta Q + \Delta W$.
 - (2) In an isolated system the entropy does not decrease.
Thus if during some process a system absorbs heat ΔQ , then its entropy changes by $\Delta S = \Delta Q/T + \Delta S_{\text{internal}} \geq \Delta Q/T$.
 - (3) The entropy at absolute zero temperature is zero (or can be set zero).

[Bookwork]

- (b) (i) Free energies are the Legendre transforms of the energy. {2}
- (ii) The free energy of a system does not increase, so at stable equilibrium it is minimal. {2}

An example: (canonical ensemble:) a system is kept at fixed temperature T while undergoing some change.

Its change in energy: $\Delta E = \Delta Q$.

Its change in entropy: $\Delta S = \Delta Q/T + \Delta S_{\text{internal}} \geq \Delta Q/T$

The relevant free energy is the Helmholtz free energy: $A(T) = E - T S$.

The change in Helmholtz free energy: $\Delta A = \underbrace{\Delta E}_{\Delta Q} - \underbrace{T \Delta S}_{\geq \Delta Q} \leq 0$. {3}

- (iii) The probability of a macroscopic state (sum of Boltzmann factors) can be expressed by a single Boltzmann factor, in which the energy is replaced by the appropriate free energy. {1}

Example: in a grand canonical ensemble the probabilities multiplied by Ξ :

$$\Xi = \sum_i e^{-\beta(E_i - \mu N_i)} = \sum_{N=0}^{\infty} e^{\beta \mu N} \underbrace{\sum_j e^{-\beta E_{j;N}}}_{\text{state with same } N} = \sum_{N=0}^{\infty} e^{-\beta(A(T;N) - \mu N)} \quad \{2\}$$

[Bookwork]

(c) (i) The partition function:

$$Z = \frac{1}{h^2} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \times \exp \left[-\beta \left(\frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{mg}{2\ell} (x^2 + y^2) \right) \right] \quad \{2\}$$

$$= \frac{1}{h^2} \underbrace{\int_{-\infty}^{\infty} dx e^{-\beta \frac{mg}{2\ell} x^2}}_{\sqrt{\frac{2\pi\ell}{\beta mg}}} \int_{-\infty}^{\infty} dy e^{-\beta \frac{mg}{2\ell} y^2} \times \underbrace{\int_{-\infty}^{\infty} dp_x e^{-\beta \frac{1}{2m} p_x^2}}_{\sqrt{\frac{2\pi m}{\beta}}} \int_{-\infty}^{\infty} dp_y e^{-\beta \frac{1}{2m} p_y^2} = \frac{\ell}{h^2 g \beta^2} \quad \{3\}$$

(ii) Average energy:

$$\langle E \rangle = -\frac{\partial \ln Z}{\partial \beta} = -\frac{\partial}{\partial \beta} \ln \frac{1}{\beta^2} = \frac{2}{\beta} = 2k_B T \quad \{3\}$$

(iii) Each quadratic half-degree of freedom (eg. $\frac{p_x^2}{2m}$ or $\frac{mgx^2}{2\ell}$) contributes $\frac{1}{2}k_B T$ to the average energy. {2}

In this case we have 4 such quadratic contributions, leading to $\langle E \rangle = 2k_B T$. {1}

[Unseen] in this form, though harmonic oscillator was covered in lecture.