STATISTICAL MECHANICS OF COMPLEX SYSTEMS – SOLUTIONS 2010

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1. (a) The thermodynamic limit of a system is the limit of infinite size (eg. infinite number of particles). $\{\mathbf{2}\}$

In the thermodynamic limit the fluctuating quantities of statistical mechanics become definite values, corresponding to thermodynamics. $\{\mathbf{2}\}$

[Bookwork]

(b) Suppose X_i are independent, identically distributed random variables with finite mean and finite variance: $\langle X_i \rangle = \mu$, and $\mathrm{Var}(X_i) = \sigma^2$, and we will consider the sum of n of these random variables. Then according to the central limit theorem

$$\frac{(X_1 + \ldots + X_n) - n\mu}{\sqrt{n}\sigma} \xrightarrow{D} \mathcal{N}(0, 1)$$

where $\mathcal{N}(0, 1)$ is the standard normal (Gaussian) distribution (zero mean, unit variance); and the convergence is in distribution (implying convergence of the cumulative distribution function, not the probability distribution function). $\{\mathbf{4}\}$

[Bookwork]

(c) (i) Denote the linear progress of the ant in one second as X_1. Then X_1 is 0 with probability $\frac{1}{2}$, 1 with probability $\frac{1}{2} \cdot \frac{7}{8}$, and -3 with probability $\frac{1}{2} \cdot \frac{1}{8}$. Then:

$$\langle X_1 \rangle = \frac{1}{2} \cdot \frac{7}{8} - \frac{1}{2} \cdot \frac{1}{8} \cdot 3 = \frac{1}{4} \text{ cm} \qquad \{\mathbf{2}\}$$

$$\langle X_1^2 \rangle = \frac{1}{2} \cdot \frac{7}{8} + \frac{1}{2} \cdot \frac{1}{8} \cdot 9 = 1 \text{ cm}^2$$

$$\mathrm{Var}(X_1) = \langle X_1^2 \rangle - \langle X_1 \rangle^2 = \frac{15}{16} \text{ cm}^2 \qquad \{\mathbf{2}\}$$

(ii)

$$\langle X_{3600} \rangle = 3600 \langle X_1 \rangle = 900 \text{ cm} \qquad \{\mathbf{1}\}$$

The distribution of X_{3600} will be approximately normal (Gaussian) $\{\mathbf{1}\}$
with mean 900 cm and variance $\sigma_{3600}^2 = 3600 \cdot \mathrm{Var}(X_1) = 3375 \text{ cm}^2 \approx (58 \text{ cm})^2$ $\{\mathbf{2}\}$

(iii) Since 7 m = $\langle X_{3600} \rangle - 3.4\sigma_{3600}$, it is very likely that the ant reaches the top of the hill. $\{\mathbf{2}\}$

[Unseen]

(d) (i) Suppose X_1 and X_2 belong to a family of distributions. If their linear combination also belongs to this family (up to an additive constant), then this family is called stable distribution. Using notation: whenever $X_1 \sim \mathrm{Fam}(\theta_1)$ and $X_2 \sim \mathrm{Fam}(\theta_2)$ implies $aX_1 + bX_2 \sim \mathrm{Fam}(\theta_3) + c$, then Fam is stable. $\{\mathbf{3}\}$

(ii) standard (Gaussian) distribution:

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp \frac{(x - x_0)^2}{2\sigma^2}$$

Cauchy (Lorentz) distribution:

$$f(x) = \frac{1}{\pi\gamma \left(1 + \left(\frac{x - x_0}{\gamma}\right)^2\right)}$$

Levy distribution:

$$f(x) = \sqrt{\frac{c}{2\pi}} \frac{e^{-c/2x}}{x^{3/2}}$$

$\{\mathbf{2}\}$ for each, with maximum of $\{\mathbf{4}\}$

[Bookwork]

2. (a) (i) A granular pile with slope less than the angle of repose (θ_r) is generally stable $\{\mathbf{1}\}$, while if its slope is larger than the maximum angle of stability ($\theta_{\max}$) than it is mechanically unstable $\{\mathbf{1}\}$. Between the two angle it is either stable or unstable, based on its history. $\{\mathbf{1}\}$
$\theta_r < \theta_{\max}$. $\{\mathbf{1}\}$
[Bookwork]

(ii) The side facing wind is mechanically stable, $0 < \alpha < \theta_r$. The other side regularly undergoes avalanches, so we can definitely say $\theta_r \leq \beta \leq \theta_{\max}$. (Actually $\beta \approx \theta_r$.) $\{\mathbf{3}\}$
[Unseen]

(b) (i) Granular segregation is the phenomenon when an non-homogeneous granular mixture separates into regions of different composition when subjected to shaking or flow. $\{\mathbf{3}\}$

(ii) **Either:**
A horizontally shaken tray is loaded with roughly one monolayer of the mixture of bronze spheres and poppy seeds. While the particles have roughly the same size, due to different mass and surface properties they have different coupling to the tray. During the course of shaking, alternating stripes composed of bronze particles and poppy seeds are formed, which are perpendicular to the direction of shaking. The stripes coarsen in time.
or:
A container, filled with water and a mixture of equal size glass and bronze spheres, is subject to vertical shaking. During the coarse of shaking, regions composed of purely glass and purely bronze are formed. Eventually only two layers are formed, paradoxically the heavier bronze particles end up in the top layer, while glass particles in the bottom layer.
$\{\mathbf{3}\}$ for either case.

(iii) One possible driving mechanism is "differential acceleration": two types of particles, initially mixed, is subject so some condition which makes the two types oscillate with at different amplitude. In a mixed state nearby particles oscillate with different amplitude, there are lots of collisions, so in an abstract phase space the system is "scattered out" from these states. However, when it encounters a segregated state, nearby particles move together, reducing the number of collisions, so there states are relatively stable. $\{\mathbf{2}\}$

[Bookwork]

(c) (i) Edwards' ensemble is the ensemble of static granular packing satisfying mechanical equilibrium (both in bulk and an the boundaries). $\{\mathbf{2}\}$
[Bookwork]

(ii) partition function:

$$Z(X) = \sum_i \exp\left(-\frac{V_i}{k_E X}\right) \qquad \{\mathbf{2}\}$$

probability of state i:

$$p_i = \frac{1}{Z(X)} \exp\left(-\frac{V_i}{k_E X}\right) \qquad \{\mathbf{2}\}$$

[Bookwork]

(iii) The lowest possible volume, corresponding to $X = 0$, is $V_{\min} = N v_0$. $\{\mathbf{2}\}$

The highest possible volume achievable in equilibrium state of an Edwards' ensemble is when all single-particle states have equal probability:
$V_{\text{max}} = N(v_0 + v_1 + v_2)/3$; the corresponding compactivity is $X = \infty$. $\{\mathbf{2}\}$
[Bookwork/Unseen]

3. (a) (i) The Legendre transform of $f(x)$ is defined as $f^*(p) = \max_x(px - f(x))$. $\{\mathbf{2}\}$
If $f(x)$ is differentiable, then the above maximum is achieved when $p(x) = df/dx$ (the differential evaluated at x). Taking its inverse function $x(p)$, the Legendre transform becomes $f^*(p) = px(p) - f(x(p))$. $\{\mathbf{2}\}$
[Bookwork]

(ii) Since the Legendre transform of the Legendre transform gives back the original function: $f^{**}(x) = f(x)$, the Legendre transform is its own inverse. $\{\mathbf{2}\}$
[Bookwork]

(iii) $p = dx^4/dx = 4x^3$, so $x(p) = (p/4)^{1/3}$. $\{\mathbf{2}\}$
Then

$$f^*(p) = px(p) - (x(p))^4 = 3\left(\frac{p}{4}\right)^{4/3} \qquad \{\mathbf{2}\}$$

[Unseen]

(b) (i) $\lambda_1, \ldots, \lambda_m$ are the Lagrange multipliers corresponding to the constraints, f_k are the constraint functions, which are evaluated at the ith state of the random variable, x_i. There are m constraints, and the random variable has n states. $\{\mathbf{2}\}$

(ii) The probability of the ith state:

$$p_i = \frac{1}{Z} \exp\left(-\sum_{k=1}^{m} \lambda_k f_k(x_i)\right) \qquad \{\mathbf{1}\}$$

The maximum value of the information entropy (the information entropy evaluated at these probabilities):

$$\begin{aligned} S(F_1, \ldots, F_m) \equiv H_{\text{max}} &= -\sum_{i=1}^{n} p_i \ln p_i = -\sum_{i=1}^{n} p_i \left(-\ln Z - \sum_{k=1}^{m} \lambda_k f_k(x_i)\right) \\ &= \ln Z \underbrace{\sum_{i=1}^{n} p_i}_{1} + \sum_{k=1}^{m} \lambda_m \underbrace{\sum_{i=1}^{n} p_i f_k(x_i)}_{\langle f_k(X)\rangle = F_k} \\ &= \ln Z(\lambda_1, \ldots, \lambda_m) + \sum_{k=1}^{m} \lambda_k F_k \qquad \{\mathbf{3}\} \end{aligned}$$

Using the definition in 3(a)(i) above, S and $-\ln Z$ are (multidimensional) Legendre transforms of each other.

(iii)

$$\begin{aligned} \langle f_k(X)\rangle &= \sum_{i=1}^{n} p_i f_k(x_i) = \sum_{i=1}^{n} \frac{1}{Z} f_k(x_i) \exp\left(-\sum_{k=1}^{m} \lambda_k f_k(x_i)\right) \qquad \{\mathbf{1}\} \\ &= \sum_{i=1}^{n} \frac{1}{Z} \frac{-\partial}{\partial \lambda_k} \exp\left(-\sum_{k=1}^{m} \lambda_k f_k(x_i)\right) = -\frac{1}{Z}\frac{\partial Z}{\partial \lambda_k} = -\frac{\partial \ln Z}{\partial \lambda_k} \qquad \{\mathbf{2}\} \end{aligned}$$

(iv) Taking the second derivative of $-\ln Z$, and changing the order of differentiation:

$$\frac{\partial \langle f_k(X)\rangle}{\partial \lambda_j} = -\frac{\partial^2 \ln Z}{\partial \lambda_j \partial \lambda_k} = -\frac{\partial^2 \ln Z}{\partial \lambda_k \partial \lambda_j} = \frac{\partial \langle f_j(X)\rangle}{\partial \lambda_k} \qquad \{\mathbf{2}\}$$

(v)

$$\mathrm{Var}(A) = \langle [A - \langle A \rangle]^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2 \qquad \{\mathbf{1}\}$$

$$\begin{aligned} \mathrm{Var}(f_j(X)) &= \langle f_j(X)^2 \rangle - \langle f_j(X) \rangle^2 \\ &= \frac{1}{Z} \frac{\partial^2 Z}{\partial \lambda_j^2} - \left(\frac{1}{Z} \frac{\partial Z}{\partial \lambda_j} \right)^2 = \frac{\partial^2 \ln Z}{\partial \lambda_j^2} \end{aligned} \qquad \{\mathbf{2}\}$$

Since the variance is an average of a square, it is non-negative, so the second derivative of $\ln Z$ is non-negative. Therefore $\ln Z$ is convex function, so its Legendre transform is well defined. $\{\mathbf{1}\}$

[Bookwork]