UNIVERSITY OF CALIFORNIA BERKELEY
Department of Civil Engineering
Fall 2010

Structural Engineering,
Mechanics and Materials
Professor: S. Govindjee

HW 3: Due September 24

1. (Micro-canonical phase space density). Consider the fundamental expression for the micro-canonical phase space density for a system with energy E (with tolerance Δ)

$$\rho = \begin{cases} \frac{1}{V(E+\Delta)-V(E)} & E \leq H(\boldsymbol{y}) \leq E+\Delta \\ 0 & \text{otherwise}\,. \end{cases}$$

Show that this can be written (for small Δ) as:

$$\rho = \begin{cases} \frac{1}{\Omega(E)\Delta} & E \leq H(\boldsymbol{y}) \leq E+\Delta \\ 0 & \text{otherwise}\,. \end{cases}$$

2. Consider an *isolated* 1-dimensional harmonic oscillator with the following Hamiltonian

$$H(p,x) \;=\; \frac{1}{2m}p^2 + \frac{1}{2}kx^2\,, \tag{1}$$

where $m = 2$ is the mass of the system and $k = 2$ is the spring constant in consistent units.

   (a) The phase-space density is given by

$$\rho = \begin{cases} \frac{1}{V(E+\Delta)-V(E)} & E \leq H(\boldsymbol{y}) \leq E+\Delta \\ 0 & \text{otherwise}\,. \end{cases}$$

   For the 1-D harmonic oscillator, in the 2-dimensional phase-space, it is known that the ensemble occupies an ellipse. What is the phase-space density for the system given by (1)? Δ will be a parameter in your result.

   (b) Determine the structure function for this system.

   (c) Determine the mean momentum of a replica in the ensemble.

   (d) In class, it was mentioned that the phase-space density ρ of an isolated Hamiltonian system is constant per unit volume in phase-space (on the constant energy ellipse) but is not constant per unit area (on the constant energy ellipse) . Assume that $H = 1$ and consider that the ellipse is given by the polar co-ordinates $(x, p) = (2\cos(\theta), \sin(\theta))$. Plot, the density per unit length of the ellipse. Is the statement from class correct or incorrect?

3. (Alternate form of the structure function). If we denote the Heaviside step function by $\Theta(\cdot)$, then the phase space volume contained within the hypersurface with energy E is

$$V(E) = \int_{\Gamma} \Theta(E - H(\boldsymbol{y}))d\boldsymbol{y}\,.$$

Determine an expression for the structure function $\Omega(E)$ in terms of the delta function. [Hint: this problem is virtually trivial.]

4. The logarithm of the phase space density is known as the index of probability, η, where

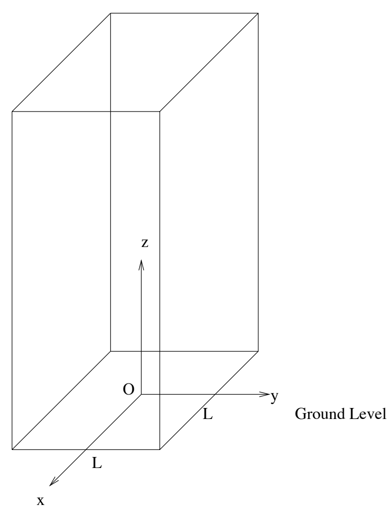
$$\eta = \log(\rho) .$$

Consider a micro-canonical ensemble and show that the phase space average of $-\eta$ is simply $\overline{-\eta} = \log(\Omega(E)\Delta)$. Thus the expectation value of the negative of the index of probability is the logarithm of the accessible phase space volume. This then is a (logarithmic) measure of how much variability in state (uncertainty) exists in the micro-canonical ensemble. As we shall see later, $\overline{-\eta}$ is intimately related to the concept of entropy.

5. Consider a point mass m with position $\boldsymbol{r} = x\boldsymbol{e}_x + y\boldsymbol{e}_y + z\boldsymbol{e}_z$, where its height above the ground is $z = \boldsymbol{r} \cdot \boldsymbol{e}_z$. The total energy of this particle is given by

$$H(\boldsymbol{r}, \boldsymbol{p}) = \frac{\boldsymbol{p} \cdot \boldsymbol{p}}{2m} + mgz , \tag{2}$$

where $\boldsymbol{p}$ is the momentum vector and g is the acceleration due to gravity. Implicit, in this expression is the constraint that $z \geq 0$ and that $x, y \in (-L/2, L/2)$.



Assume a canonical phase-space distribution for this particle given by

$$\rho(\boldsymbol{r}, \boldsymbol{p}) = C \exp(-\frac{H}{k_B T}) , \tag{3}$$

where $k_B = 1.3806504 \times 10^{-23}$ J/K is Boltzmann constant, T is the absolution temperature of the surroundings (the heat bath) and C is the normalization constant.

(a) Calculate the mean height of the particle above the ground? Express it in terms of m, g, k_B and T.

(b) Assume the particle is a Helium atom with mass $4.0026/N_A$ g and the surrounding temperature is 300 K. What is the mean height? [Note: $N_A = 6.022 \times 10^{23}$ is Avagadro's number.]

(c) Assume that the particle has mass 10 kg and the surrounding temperature is 300 K. What is the mean height now? Does this correlate with your physical intuition?

Useful integrals:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\frac{\pi}{\alpha}}$$

$$\int_{0}^{\infty} e^{-\alpha x^2} dx = \frac{1}{2}\sqrt{\frac{\pi}{\alpha}}$$

$$I(n) = \int_{0}^{\infty} e^{-\alpha x^2} x^n dx = \frac{1}{2}\Gamma\left(\frac{n+1}{2}\right)\alpha^{-(n+1)/2} = -\frac{\partial I(n-2)}{\partial \alpha}$$

The gamma-function:

$$\begin{aligned} \Gamma(n) &= (n-1)\Gamma(n-1) = (n-1)! \\ \Gamma(1) &= 1 \\ \Gamma(1/2) &= \sqrt{\pi} \end{aligned}$$

The error-function:

$$\mathrm{erf}(y) = \frac{2}{\sqrt{\pi}} \int_0^y e^{-x^2} dx$$

Stirling's formula:

$$n! = \sqrt{2\pi n}\; n^n e^{-n} \left[1 + \frac{1}{12n} + \cdots\right] \qquad \text{for } n \gg 1\,.$$

Thus for $n > 10$ the error in using only the pre-factor is already only 1 percent. For very large n , $\ln(n) \ll n$, this reduces to $\ln(n!) \approx n\ln(n) - n$.

Useful expression for the Kronecker-Delta:

$$\delta_{nm} = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{i(n-m)\theta} d\theta$$

Useful expressions for the Dirac-Delta function:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-ikx} dk\,.$$

This expression simply comes from the inverse Fourier transform expression for the delta function.