5. Integrated density of states

The number of accessible states, $\Omega(E)$, is defined as the number of states with energies between $E - \Delta E$ and $E$. Alternatively, we can define $\tilde{\Omega}_x(E)$ as the number of states with energies between $xE$ and $E$, where $0 \leq x \leq 1$. For a classical system, 

$$\tilde{\Omega}_x(E) = \text{const.} \times \int_{xE \leq H \leq E} d\Gamma,$$

where $d\Gamma = d^3x_1 \ldots d^3x_N \, d^3p_1 \ldots d^3p_N$ is the phase space volume element, and $H$ is the energy of a microstate. The normalization constant will be of no relevance for what follows. $\tilde{\Omega}_{x=0}(E)$ is called the integrated density of states.

a) For a classical ideal gas ($N$ noninteracting point particles of mass $m$ in a volume $V$), show that 

$$\tilde{\Omega}_{x=0}(E) = \text{const.} \times V^N \left(2mE\right)^{3N/2} C_{3N},$$

with $C_d$ the volume of the $d$-dimensional unit sphere. Calculate $C_d$.

b) Show that 

$$\tilde{\Omega}_x(E) = f(x) \tilde{\Omega}_0(E),$$

and determine $f(x)$. How close to 1 do you have to choose $x$ in order for $f(x)$ to be substantially different from unity? Discuss the meaning of this result for the volumes of high-dimensional spheres, and for the physical significance of the arbitrary energy interval $\Delta E$ in the number of accessible states.

(7 points)

6. Particle in a box

Consider a quantum mechanical system consisting of one spinless particle in a 3-dimensional rectangular box with linear dimensions $L_1$, $L_2$, and $L_3$.

a) Suppose the system is in a particular microstate. From the change of the corresponding energy level under a quasi-static change of the length $L_i$ by $dL_i$, find the force exerted by the particle on the wall perpendicular to the $i$-axis.

b) For a cubic box, find the average pressure of the particle on a wall in terms of the average energy of the particle and the volume of the box.

hint: You do not need to find the probability distribution explicitly.

(4 points)
7. Energy fluctuations

Consider a canonical ensemble with partition function $z$.

a) Show that the mean energy and the root-mean-square deviation of the energy are given by

$$U = \langle E \rangle = - \frac{\partial \log Z}{\partial \beta}$$

$$\langle \Delta E \rangle = \left\langle (E - \langle E \rangle)^2 \right\rangle^{1/2} = \left( \frac{\partial^2 \log Z}{\partial \beta^2} \right)^{1/2}$$

b) Show that the energy distribution function is Gaussian,

$$\rho(E) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\langle \Delta E \rangle^2 / \sigma^2}$$

where the standard deviation is small of order

$$\sigma^2/U^2 = O(1/N)$$

**hint:** Divide the system into a large number of identical subsystems that are still macroscopic and each have canonical distribution, and use the central limit theorem.

(7 points)
5. a) Constant 4e \Rightarrow H = \frac{1}{\epsilon} \sum p_i \frac{1}{r_i}

\Rightarrow \tilde{R}_{x=0}(E) = \sum p_i \int dx_1 dx_3 \int dx_3 \int dp_1 \int dp_3 \int dp_{2N} \Theta(E - \frac{1}{\epsilon} \sum p_i \frac{1}{r_i})

= \sum p_i \int dp_1 \int dp_3 \int dp_{2N} \Theta(E - \frac{1}{\epsilon} \sum p_i)

= \sum p_i \int \frac{1}{2N} \frac{1}{2N} \frac{1}{2N} \int dx_1 dx_3 \int dp_1 \int dp_3 \int dp_{2N} \Theta(1 - \frac{1}{\epsilon} \sum p_i)

= \sum p_i \int \frac{1}{2N} \frac{1}{2N} \frac{1}{2N} \int dx_1 dx_3 \int dp_1 \int dp_3 \int dp_{2N} \Theta(1 - \frac{1}{\epsilon} \sum p_i)

\Rightarrow \forall \epsilon \quad C_0 = \int dx_1 dx_3 \Theta(1 - \epsilon x_i) = \text{volume of } d\text{-chain unit sphere}

\text{sphere of radius } r \quad V_d(r) = C_d r^d \quad \text{volume}

S_d(r) = \frac{d - 1}{d} C_d r^d \quad \text{surface area}

Consider

\Rightarrow F_d = \int dx_1 dx_3 e^{-\epsilon(x_1^2 + \cdots + x_3^2)} \left( \int dx e^{-\epsilon x^2} \right)^d = (\pi/e)^{d/2}

= \int dr \int dx_1 x_1 e^{-\epsilon r^2} = \frac{d}{d-1} C_d \int dr r^{d-1} e^{-\epsilon r^2}

= \frac{d}{d-1} C_d e^{-\epsilon r^2} \left( \frac{d}{d-1} + 1 \right)

\Rightarrow C_d = \frac{\pi}{\alpha} \frac{d}{d-1} + 1

b) Consider a diminished sphere of radius \( r \), and a spherical shell of thickness \( (1-x)r \). The shell volume is

\Rightarrow V_{shell}(x) = V_d(r) - V_d(xr) = \frac{C_d}{2N} \left[ r^d - (xr)^d \right] - \frac{V_d(r)}{[1-x]^d]
\[ \tilde{R}_x(x) = \tilde{R}_0(x)(1 - x^{2N}) = f(x) \tilde{R}_0(x) \]

\[ f(x) = 1 - x^{2N} \]

Happen we want a 10% difference between \( \tilde{R}_x \) and \( \tilde{R}_0 \).

\[ f(x) = 0.99 = 1 - x^{2N} \]

\[ x^{2N} = 0.01 \]

\[ x = (0.01)^{1/2N} = 10^{-2/N} \approx 10^{-10^{-22}} \]

Conclude:
1. For high-dimensional spheres, almost all of the volume bits are essentially thin shells near the surface.
2. \( x \) must be ridiculously close to 1 for \( \tilde{R}_x \) to be meaningfully different from \( \tilde{R}_0 \).
3. For macroscopic systems, no meaningful physical property can depend on the bin of the arbitrary mass spread \( AE \).
6) a) When we consider the energy spectrum of
\[ E_m = \left( \frac{k \hbar c}{2m} \right)^2 \left( \frac{1}{l_i / \hbar c} \right)^2 \]
when \( m \) is the particle mass, and \( n_i = 0, 1, 2, \ldots (i = 1, 2) \)

b) The form energy to achieve this shape is
\[ E \frac{\partial}{\partial r} \cong \frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} - \frac{\hbar^2}{2m} \frac{n_i}{L_i} \]

For a particle in a 2, 3-vell.
\[ p = \langle F_s \rangle / L_2 L_3 = \frac{\hbar^2}{2m} \frac{\langle F_s \rangle}{L_2 L_3} = \frac{\hbar^2}{2m} \frac{\langle \Delta s \rangle}{L_2 L_3} \]

For a 3-vell, \( \langle \Delta s \rangle = \langle n_i^2 \rangle = \langle n_i^2 \rangle + \langle n_i \rangle \), and \( n_i = 0, 1, 2 \)

\[ \langle E \rangle = \frac{\hbar^2}{2m} \left( \frac{\langle \Delta s \rangle^2}{L_2^2} + \frac{\langle \Delta s \rangle}{L_2} + \frac{\langle \Delta s \rangle}{L_2} \right) = \frac{\hbar^2}{2m} \frac{\langle \Delta s \rangle^2}{L_2^2} \]

\[ p = \frac{\hbar d}{2} \frac{d}{2} \frac{d}{2} \frac{d}{2} \]
1) a) \[ t = \frac{E}{e^{-AE}} \] is a canonical partition function.

\[ \frac{\partial \ln t}{\partial A} = \frac{1}{E} \frac{E - AE}{E} = \langle E \rangle \]

\[ \frac{\partial^2 \ln t}{\partial A^2} = \frac{-2}{E^2} \left( \frac{1}{E} E e^{-AE} \right) + \frac{1}{E^2} \left( E e^{-AE} \right) \frac{\partial E}{\partial A} + \frac{1}{E} \frac{E}{E} e^{-AE} \]

\[ = \langle E^2 \rangle - \langle E \rangle \frac{\partial \ln t}{\partial A} = \langle E^2 \rangle - \langle E \rangle^2 = (\Delta E)^2 \]

b) Divide the system into subsystems and marginalize \( E \): \( \{ i = 1, \ldots, n \} \)

\[ E = E_i \]

The \( E_i \) are random variables.

Each of \( E_i \) is governed by a canonical distribution with partition function \( t_i = \frac{E_i}{e^{-AE_i}} \)

with \( E_i \) the energy levels of subsystem \( i \).

The subsystems are identical \( \Rightarrow t_i = t \Rightarrow t = x_i \)

The canonical distribution loss e Gaußian variance.

Now consider the CLT in the form

**CLT:** Let \( X_i (i = 1, \ldots, N) \) be \( N \) independent random variables

with \( \langle X_i \rangle, \langle X_i^2 \rangle < \infty \), let \( t = \frac{1}{N} \sum X_i \).

For \( N \to \infty \) \( t \) loss e Gaussian PDF

\[ \phi(t) = \frac{1}{\sqrt{2\pi \sigma^2}} e^{-\frac{(t-\mu)^2}{2\sigma^2}} \]
All premises are fulfilled \( \Rightarrow \) The CLT applies with

\[ X_i = NE_i, \quad z = E \]

\[ f(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{(z-E)^2}{2\sigma^2}} \]

and

\[ \frac{1}{\sqrt{2\pi}} \sum_{i=1}^{n} (X_i - \langle X_i \rangle)^2 = n (\Delta E)^2 = n \frac{\partial^2 \log z}{\partial \Delta^2} = \frac{1}{\partial \Delta^2} \]

Hence, the specific heat is

\[ C_v = \left( \frac{\partial u}{\partial T} \right)_v = -\frac{\Delta}{\Delta} \frac{\partial u}{\partial \Delta} = \frac{\Delta}{\Delta} (\Delta E)^c \]

and for a macroscopic system we have

\[ C_v = 0 (N \hbar^2) \quad \text{and} \quad U = 0 (N \hbar^2 \Delta) \]

\[ \frac{\Delta^2}{u^2} = \frac{(\Delta E)^c}{u^2} = \frac{\Delta^2}{u^2} C_v = 0 \left( \frac{\hbar^2 \Delta^2}{N} \right) = 0 (1/N) \]