Problem Assignment # 2

04/07/2022
due 04/14/2022

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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,

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

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

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

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

b) Show that

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

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 ΔE 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)

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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

$$U = \langle E \rangle = -\partial \log Z / \partial \beta$$

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

b) Show that the energy distribution function is Gaussian,

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

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) Classical ideal gas $\rightsquigarrow$ $H = \sum_{i=1}^{3N} p_i^2/2m$

$$\rightsquigarrow \underline{\tilde{\Omega}_{x=0}(E)} = \text{const} \times \int dx_1 \dots dx_{3N} \int dp_1 \dots dp_{3N}\ \Theta\left(E - \sum_{i=1}^{3N} p_i^2/2m\right)$$

$$= \text{const} \times V^{3N} \int dp_1 \dots dp_{3N}\ \Theta\left(2mE - \sum_{i=1}^{3N} p_i^2\right)$$

$$= \text{const} \times V^{3N} (2mE)^{3N/2} \int d\pi_1 \dots d\pi_{3N}\ \Theta\left(1 - \sum_{i=1}^{3N} \pi_i^2\right)$$

$$= \underline{\underline{\text{const} \times V^{3N} (2mE)^{3N/2}\, C_{3N}}}$$

1 with $\underline{C_d = \int dx_1 \dots dx_d\ \Theta\left(1 - \sum_{i=1}^{d} x_i^2\right)}$ = volume of d-dim. unit sphere

sphere of radius r: $V_d(r) = C_d r^d$ volume

$S_d(r) = d\, C_d\, r^{d-1}$ surface area

1

Consider

$$\underline{Z_d} := \int dx_1 \dots dx_d\ e^{-a(x_1^2 + \dots + x_d^2)} = \left(\int dx\, e^{-ax^2}\right)^d = \underline{(\pi/a)^{d/2}}$$

$$= \int_0^\infty dr\ S_d(r)\ e^{-ar^2} = d\, C_d \int_0^\infty dr\, r^{d-1} e^{-ar^2}$$

$$= \tfrac{1}{2} d\, C_d \int_0^\infty dx\, x^{\frac{d-2}{2}} e^{-ax} = \tfrac{1}{2} d\, C_d\, a^{-d/2} \int_0^\infty dx\, x^{\frac{d}{2}-1} e^{-x}$$

$$= \tfrac{1}{2} d\, C_d\, a^{-d/2}\, \Gamma(d/2) = \underline{C_d\, a^{-d/2}\, \Gamma(d/2+1)}$$

$$\rightsquigarrow \underline{\underline{C_d = \pi^{d/2} / \Gamma(d/2+1)}}$$

1

b) Consider d-dimensional sphere of radius r, and a spherical shell of thickness $(1-x)r$ $\rightsquigarrow$ The shell volume is

$$\underline{V_{shell}(x)} = V_d(r) - V_d(xr) = C_d\left[r^d - (xr)^d\right] = \underline{V_d(r)\left[1 - x^d\right]}$$

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$$\rightarrow \underline{\underline{\tilde{\Omega}_x(E)}} = \tilde{\Omega}_0(E)\,(1-x^{3N}) = \underline{\underline{f(x)\,\tilde{\Omega}_0(E)}}$$

with $\underline{\underline{f(x) = 1-x^{3N}}}$

1

Suppose we want a 1% difference between $\tilde{\Omega}_x$ and $\tilde{\Omega}_0$.

$$\rightarrow f(x) \overset{!}{=} 0.99 = 1-x^{3N}$$

$$\rightarrow x^{3N} = 0.01$$

$$\rightarrow \underline{\underline{x}} = \left(\frac{1}{100}\right)^{1/3N} = 10^{-2/3N} \sim \underline{\underline{10^{-10^{-22}}}}$$

1

conclusion: (1) For high-dimensional systems, almost all of the volume sits in extremely thin shell near the surface.

(2) x must be ridiculously close to 1 for $\tilde{\Omega}_x$ to be meaningfully different from $\tilde{\Omega}_0$.

(3) For macroscopic systems, no meaningful physical property can depend on the size of the arbitrary energy interval ΔE

1

6) a) QM ~> the energy spectrum is

$$E_{[n_i]} = \frac{(\hbar\pi)^2}{2m} \sum_{i=1}^{3} (n_i/L_i)^2$$

(1) where m is the particle mass, and $n_i = 0, 1, 2, \ldots$ $(i=1,\ldots$

Consider $i=1$ w.l.g. Let $L_1 \to L_1 + dL_1$ quasi-statically

$$\rightsquigarrow \frac{\partial E_{[n_1,n_2,n_3]}}{\partial L_1} = -\frac{\hbar^2\pi^2}{2m}\frac{n_1^2}{L_1^3}$$

~> the force necessary to achieve this change is

(1) $$\underline{\underline{F_1}} = -\frac{\partial E}{\partial L_1} = \underline{\underline{\frac{\hbar^2\pi^2}{m}\frac{n_1^2}{L_1^3}}}$$ force exerted on the 2,3-wall

b) Macroscopic pressure on the 2,3-wall:

(1) $$\underline{p} = \langle F_1\rangle / L_2L_3 = \frac{\hbar^2\pi^2}{m}\frac{\langle n_1^2\rangle}{L_1^3L_2L_3} \overset{\text{cube}}{=} \underline{\frac{\hbar^2\pi^2}{m}\frac{\langle n_1^2\rangle}{L^5}}$$

That for a cube, $\langle n_1^2\rangle = \langle n_2^2\rangle = \langle n_3^2\rangle$, and so

$$\langle E\rangle = \underline{U} = \frac{\hbar^2\pi^2}{2m}\left(\frac{\langle n_1^2\rangle}{L_1^2} + \frac{\langle n_2^2\rangle}{L_2^2} + \frac{\langle n_3^2\rangle}{L_3^2}\right) = \underline{\frac{3\hbar^2\pi^2}{2m}\frac{\langle n_1^2\rangle}{L^2}}$$

(1) $$\rightsquigarrow \underline{\underline{p}} = \frac{2}{3}U/L^3 = \underline{\underline{\frac{2}{3}U/V}}$$

2.) a) $Z = \sum_n e^{-\beta E_n}$ canonical partition fct.

$$\rightsquigarrow \underline{\underline{\frac{-\partial \log Z}{\partial \beta}}} = \frac{1}{Z}\sum_n E_n e^{-\beta E_n} = \underline{\underline{\langle E \rangle}}$$

$$\underline{\frac{\partial^2 \log Z}{\partial \beta^2}} = \frac{-\partial}{\partial \beta}\left(\frac{1}{Z}\sum_n E_n e^{-\beta E_n}\right) = \frac{1}{Z^2}\left(\sum_n E_n e^{-\beta E_n}\right)\frac{\partial Z}{\partial \beta} + \frac{1}{Z}\sum_n E_n^2 e^{-\beta E_n}$$

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$$= \langle E^2 \rangle - \langle E \rangle \frac{-\partial \log Z}{\partial \beta} = \langle E^2 \rangle - \langle E \rangle^2 = \underline{\underline{(\Delta E)^2}}$$

b) Divide the system into n subsystems with energies e_i $(i = 1, \dots, n)$

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$$\rightsquigarrow E = \sum_i e_i$$

The e_i are random variables.

each of which is governed by a canonical distribution with partition fct. $Z_i = \sum_m e^{-\beta \varepsilon_m^{(i)}}$

with $\varepsilon_m^{(i)}$ the energy levels of subsystem # i.

The subsystems are identical $\rightsquigarrow Z_i \equiv Z$ and $Z = Z^n$

1

The canonical distribution has a finite variance.

Now consider the CLT in the form

<u>CLT</u>: Let X_i $(i = 1, \dots, N)$ be N independent random variables with $\langle X_i \rangle, \langle X_i^2 \rangle < \infty$. Let $\underline{y} = \frac{1}{N}\sum_i X_i$. Then for $N \to \infty$ $\underline{y}$ has a Gaussian pdf

$$\boxed{\rho(y) = \frac{1}{\sqrt{2\pi}\,\sigma} e^{-(y - \langle y \rangle)^2/2\sigma^2}} \quad \text{with } \sigma^2 = \frac{1}{N^2}\sum_{i=1}^{N}\langle (X_i - \langle X_i \rangle)^2 \rangle$$

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All premises are fulfilled $\rightarrow$ the CLT applies with

$$x_i = N\varepsilon_i \ , \ y = E$$

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

(1)

with $\underline{\sigma^2} = \sum_{i=1}^{n} \langle (\varepsilon_i - \langle \varepsilon_i \rangle)^2 \rangle = n(\Delta\varepsilon)^2 \overset{a)}{=} n \frac{\partial^2 \log Z}{\partial \Lambda^2} =$

$$= \frac{\partial^2 \log Z}{\partial \Lambda^2} = \underline{(\Delta E)^2}$$

(1)

But the specific heat is

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V = -\frac{\Lambda}{T}\frac{\partial U}{\partial \Lambda} \overset{a)}{=} \frac{\Lambda}{T}(\Delta E)^2$$

(1)

and for a macroscopic system we have $C_V = O(N k_B)$

and $U = O(N k_B T)$

$$\rightarrow \quad \underline{\frac{\sigma^2}{U^2}} = \frac{(\Delta E)^2}{U^2} = \frac{k_B T^2 C_V}{U^2} = O\left(\frac{k_B^2 T^2 N}{k_B^2 T^2 N^2}\right) = \underline{\underline{O(1/N)}}$$

(1)