1. Maximize the Gibbs entropy (with $k_B = 1$) subject to the constraints

$$\langle x \rangle = \sum_i x_i p(x_i) \quad (1)$$
$$\langle x^2 \rangle = \sum_i x_i^2 p(x_i), \quad (2)$$

to find the probability distribution of x_i. Here, $p(x_i)$ is the probability of x_i. Show that this becomes the normal distribution when x is allowed to be continuous and run from $-\infty$ to ∞, i.e.

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

with $\mu = \langle x \rangle$ and $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$. Note that for continuous x, $p(x)$ is a probability density, so that the normalization condition is given by $\int_{-\infty}^{\infty} dx\, p(x) = 1$, for instance.

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Gibbs entropy: $S = -\sum_i p_i \ln p_i$. To fullfill the constraints we introduce 3 Lagrange multiplyer:

$$\mathcal{L} = \underbrace{-\sum_i p_i \ln p_i}_{S} + \lambda_0 \underbrace{\left(1 - \sum_i p_i\right)}_{\text{normalization}} + \lambda_1 \underbrace{\left(\langle x \rangle - \sum_i x_i p_i\right)}_{(1)} + \lambda_2 \underbrace{\left(\langle x^2 \rangle - \sum_i x_i^2 p_i\right)}_{(2)}$$

Maximize it: $\frac{\partial \mathcal{L}}{\partial p_i} = -\ln p_i - \lambda_0 - \lambda_1 x_i - \lambda_2 x_i^2 - 1 \stackrel{!}{=} 0$

$$\Rightarrow p_i = \exp(-\lambda_0 + \lambda_1 x_i + \lambda_2 x_i^2 - 1)$$

with (1) and (2) $\left(\frac{\partial \mathcal{L}}{\partial \lambda_i} = 0\right)$ to find $\{\lambda_i\}$

(and normalization)

Now we want $x_i \to x \in \mathbb{R}$ to be continuous.

$$\Rightarrow p_i \to p(x_i) = C \exp(-\lambda_0 + \lambda_1 x_i + \lambda_2 x_i^2 - 1)$$

so that $p_i = p(x_i)\,dx$

So: $p(x) = C \exp(-\lambda_0 + \lambda_1 x + \lambda_2 x^2 - 1) = C \exp\left(-\lambda_2 \left(x + \frac{\lambda_1}{2\lambda_2}\right)^2 + \frac{\lambda_1^2}{4\lambda_2^2} - \lambda_0\right)$

$$= \underbrace{C \exp\left(\frac{\lambda_1^2}{4\lambda_2^2} - \lambda_0\right)}_{=: C'} \exp\left(-\lambda_2 \left(x \; \frac{\lambda_1}{2\lambda_2}\right)^2\right)$$

Use constraints to find $C'(\lambda_0, \lambda_1, \lambda_2)$, λ_1 and λ_2.

First, normalization to find c':

$$\int_{-\infty}^{\infty} c' \exp\left(-\lambda_2 \left(x + \frac{\lambda_1}{2\lambda_2}\right)^2\right) dx$$

Using $u = \sqrt{\lambda_2}\left(x + \frac{\lambda_1}{2\lambda_2}\right)$

$\Rightarrow du = \sqrt{\lambda_2}\, dx$

$$= \frac{c'}{\sqrt{\lambda_2}} \underbrace{\int_{-\infty}^{\infty} \exp(-u^2)\, du}_{\sqrt{\pi}}$$

$$= c' \sqrt{\frac{\pi}{\lambda_2}} \stackrel{!}{=} 1 \quad \Rightarrow \quad c' = \sqrt{\frac{\lambda_2}{\pi}}$$

Use 1 :

$$\langle x \rangle = \int_{-\infty}^{\infty} p(x)\, x\, dx = \sqrt{\frac{\lambda_2}{\pi}} \int_{-\infty}^{\infty} x \exp\left(-\lambda_2\left(x + \frac{\lambda_1}{2\lambda_2}\right)^2\right) dx$$

Again: $u = \sqrt{\lambda_2}\left(x + \frac{\lambda_1}{2\lambda_2}\right) \Rightarrow x = \frac{u}{\sqrt{\lambda_2}} - \frac{\lambda_1}{2\lambda_2}$

$$= \pi^{-1/2} \int_{-\infty}^{\infty} \left(\frac{u}{\sqrt{\lambda_2}} - \frac{\lambda_1}{2\lambda_2}\right) \exp(-u^2)\, du$$

$\int_{-\infty}^{\infty} u\, du = 0$

$$= -\pi^{-1/2} \frac{\lambda_1}{2\lambda_2} \int_{-\infty}^{\infty} \exp(-u^2)\, du = -\sqrt{\frac{\pi}{\pi}} \frac{\lambda_1}{2\lambda_2} = -\frac{\lambda_1}{2\lambda_2} =: \mu$$

Using 2 :

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 p(x)\, dx = \sqrt{\frac{\lambda_2}{\pi}} \int_{-\infty}^{\infty} x^2 \exp\left(-\lambda_2 (x - \mu)^2\right)$$

$x = \frac{u}{\sqrt{\lambda_2}} - \frac{\lambda_1}{2\lambda_2} = \frac{u}{\sqrt{\lambda_2}} + \mu \quad = \mu^2 + 2\frac{u}{\sqrt{\lambda_2}}\mu + \frac{u^2}{\lambda_2}$

$$= \underbrace{\pi^{-1/2} \int_{-\infty}^{\infty} \exp(-u^2)}_{du\, = 1} \left(\mu^2 + \cancel{2\frac{u}{\sqrt{\lambda_2}}\mu} + \frac{u^2}{\lambda_2}\right) du$$

$\int_{-\infty}^{\infty} u \exp(-u^2)\, du = 0$ with $u' = u^2$

$$= \mu^2 + \frac{2}{\lambda_2\sqrt{\pi}} \int_{-\infty}^{\infty} u^2 \exp(-u^2)\, du = \mu^2 + \frac{2}{\lambda_2\sqrt{\pi}} \int_0^{\infty} \frac{\sqrt{u'}}{2} e^{-u'}\, du'$$

$$= \mu^2 + (\lambda_2\sqrt{\pi})^{-1}\, \Gamma\left(\frac{3}{2}\right) = \mu^2 + \frac{1}{2\lambda_2}$$

$$\sigma^2 := \langle x^2 \rangle - \langle x \rangle^2 = \langle x^2 \rangle - \mu^2 = \frac{1}{2\lambda_2} \Rightarrow \lambda_2 = \frac{1}{2\sigma^2}$$

And thus: $p(x) = (2\pi\sigma^2)^{-1/2} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$

is a Gaussian PDF!

2. Consider a system in the grand canonical ensemble with two single-particle energy states 0 and ϵ.

(a) Assuming the particles are Fermions, calculate $\langle N \rangle$ as a function of μ and T. Show the limits as $T \to 0$ and ∞.

(b) Assuming the particles are Bosons, calculate $\langle N \rangle$ as a function of μ and T. Show the limits as $T \to 0$ and ∞.

(a) Fermions

$$Z = \prod_i \left[1 + \exp(-\beta(\varepsilon_i - \mu))\right] = (1 + e^{\beta\mu})\left[1 + \exp(\beta(\mu - \varepsilon))\right]$$

$$\langle N \rangle = \left(\frac{\partial \ln Z}{\partial(\beta\mu)}\right)_T = \frac{e^{\beta\mu}}{1+e^{\beta\mu}} + \frac{\exp(\beta(\mu-\varepsilon))}{1+\exp(\beta(\mu-\varepsilon))} = \frac{1}{1+e^{-\beta\mu}} + \frac{1}{1+\exp(\beta(\varepsilon-\mu))}$$

$T \to 0$

$$\lim_{T\to 0} \exp\left(-\frac{X}{T}\right) = \begin{cases} 0, & X > 0 \\ \infty, & X > 0 \end{cases}$$

$$\Rightarrow \lim_{T\to 0} \frac{1}{1+\exp(-\frac{X}{T})} = \Theta(X)$$

$$\lim_{T\to 0} \langle N \rangle = \Theta(\mu) + \Theta(\mu - \varepsilon)$$

$T \to \infty$

$$\lim_{T\to\infty} \langle N \rangle = \frac{1}{2} + \frac{1}{2} = 1$$

(b) Bosons

$$Z = \prod_i (1 - \exp(-\beta(\varepsilon_i - \mu)))^{-1} = \left[(1 - e^{\beta\mu})(1 - \exp(-\beta(\varepsilon - \mu)))\right]^{-1}$$

$$\langle N \rangle = \left(\frac{\partial \ln Z}{\partial(\beta\mu)}\right)_T = (e^{-\beta\mu} - 1)^{-1} + (\exp(\beta(\varepsilon - \mu)) - 1)^{-1}$$

For bosons: $\mu < \min(0, \varepsilon)$

$$\lim_{T\to 0} \langle N \rangle = 0$$

$\lim_{T\to\infty} \exp\left(-\frac{X}{T}\right) = 1$, not helpful, case $\frac{0}{0}$ $\Rightarrow$ L'Hospital

$$\Rightarrow \lim_{T\to\infty} \langle N \rangle = \frac{1}{-\beta\mu} + \frac{1}{-\beta(\mu-\varepsilon)} = -\frac{T}{\mu} - \frac{T}{\mu-\varepsilon}$$

3. Consider a system with two single-particle states 1 and 2. This system could also be in the mixed states

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}}[|1\rangle \pm |2\rangle]$$

(a) Write down the density matrix for the system in the basis defined by 1 and 2 when the system is in state $|\psi_+\rangle$ and verify $\hat{\rho}^2 = \hat{\rho}$.

(b) Now consider the density matrix

$$\hat{\rho} = \sum_{a=\pm} p_a |\psi_a\rangle\langle\psi_a|.$$

$p_+ + p_- = 1$. Find the value of p_+ which minimizes the purity of the ensemble, $\mathrm{Tr}\,\hat{\rho}^2$.

(a) Assuming that the states are normalized!

$$\rho = \frac{1}{2}\left(|1\rangle\langle 1| + |1\rangle\langle 2| + |2\rangle\langle 1| + |2\rangle\langle 2|\right)$$

$$\rho_{11} = \langle 1|\rho|1\rangle = \frac{1}{2} = \rho_{12} = \rho_{21} = \rho_{22}$$

so $\rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ and $\rho^2 = \frac{1}{4}\begin{pmatrix} 2 & 2 \\ 2 & 2 \end{pmatrix} = \rho$ ✓

(b) Obviously $p_+ = p_- = \frac{1}{2}$, the maximally mixed state.

Explicitly:

$$\rho = \frac{p_+}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{p_-}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

$$\Rightarrow \rho^2 = \frac{1}{2}\begin{pmatrix} p_+^2 + p_-^2 & p_+^2 - p_-^2 \\ p_+^2 - p_-^2 & p_+^2 + p_-^2 \end{pmatrix}$$

$$\Rightarrow \mathrm{tr}(\rho^2) = p_+^2 + p_-^2$$

Maximum for $p_+ = 1, p_- = 0$ or $p_- = 1, p_+ = 0$

$$\boxed{\text{Minimum for } p_+ = p_- = \frac{1}{2}}$$

✓

✓

4. In some cases, we might want to talk about systems that have a net macroscopic angular momentum in a particular direction. If the system could exchange angular momentum and energy with the world around it, then it would be natural to describe its properties in terms of an ensemble subject to the constraints $\langle L\rangle = \sum_i p_i L_i$, $\sum_i p_i = 1$, and $\langle E\rangle = \sum_i p_i E_i$, but with every ensemble member having fixed volume V and particle number N.

Solar systems?

(a) Write down the normalized probability p_i for drawing an ensemble member in state i and define the normalization coefficient (or partition function) for this ensemble Z_L.

(b) Consider a system of N distinguishable quantum rotors that rotate about the same fixed axis, with single particle energies $\epsilon_m = \frac{\hbar^2}{2I}m^2$ and single particle angular momenta $\ell = \hbar m$, where $m = -\infty, ..., -1, 0, 1, ...\infty$. I is the moment of inertia of a single rotor. Calculate Z_L for this system (eventually assuming that the energy levels are closely spaced enough to take sums over m to integrals).

(c) Calculate the average angular momentum of the system of quantum rotors and show that the Lagrange multiplier associated with the angular momentum constraint multiplied by T can be interpreted as the net angular velocity of the system.

(d) Calculate the average energy of the system of quantum rotors.

(a)

Maximize Gibbs entropy with given constraints:
(See Problem 1)

$$\mathcal{L} = \underbrace{-\sum_i p_i \ln p_i}_{S} + \lambda_0 \underbrace{\left(1 - \sum_i p_i\right)}_{\text{normalization}} + \lambda_1\left(\langle E\rangle - \sum_i p_i E_i\right) + \lambda_2\left(\langle L\rangle - \sum_i p_i L_i\right)$$

We know that $\lambda_1 = \beta$, $\lambda_2 = \omega\beta$

$$\Rightarrow \frac{\partial \mathcal{L}}{\partial p_i} = -\ln p_i - 1 - (\lambda_0 + \beta E_i - \omega\beta L_i) \overset{!}{=} 0$$

$$\Rightarrow p_i = \exp\left(-\beta(E_i - \omega L_i)\right) \underbrace{\exp(-\lambda_0 - 1)}_{Z_L^{-1} \text{ for normalization}}$$

$$Z_L = \sum_i \exp\left(-\beta(E_i - \omega L_i)\right)$$

(b)

$$L_i = \hbar \sum_{j=1}^{N} m_{ij} \qquad E_i = \frac{\hbar^2}{2I}\sum_{j=1}^{N} m_{ij}^2$$

\# Particles in system

system/state

particle in system

Since there are N different configurations for distinguishable:

$$Z_L = \sum_{m_1} \exp(-\beta\,\mathcal{E}(m_1)) \cdots \sum_{m_N} \exp(-\beta\,\mathcal{E}(m_N)) = \left(\sum_{m=-\infty}^{\infty} \exp\left(-\beta\left(\frac{\hbar^2}{2I}m^2 - \omega\hbar m\right)\right)\right)^N$$

$$\approx \left(\int_{-\infty}^{\infty} \exp(\cdots)\,dm\right)^N = \left(\frac{2\pi I T}{\hbar^2}\right)^{N/2} \exp\left(\frac{N I \omega^2}{2T}\right)$$

(c) $\langle L \rangle = \sum_i p_i L_i = Z_L^{-1} \sum_i L_i \exp(-\beta(E_i - \omega L_i)) = T\left(\frac{\partial \ln Z_L}{\partial \omega}\right)_T$

$$= T \frac{\partial}{\partial \omega}\left(\frac{NI\omega^2}{2T} + \frac{N}{2}\ln(2\pi I T/\hbar^2)\right)$$

$$= N\omega I \Rightarrow \omega = \frac{\langle L \rangle}{NI} \quad \text{(makes sense!)}$$

(d) $\langle E \rangle = -\left(\frac{\partial \ln Z_L}{\partial \beta}\right)_{\beta\omega} = -\frac{\partial}{\partial \beta}\left(\beta\frac{NI\omega^2}{2} - \frac{N}{2}\ln\left(\frac{\beta\hbar^2}{2\pi I T}\right)\right)$

$$= \frac{NI\omega^2}{2} + \frac{NT}{2} = \frac{1}{2}(\langle L \rangle \omega + NT)$$