

SM-1 September 2016

- N non-interacting particles
 $\rightarrow$ fixed position $\rightarrow$ Distinguishable
 $\rightarrow$ magnetic moment μ

Magnetic field H

Energy states: $E=0$ or $E=2\mu H$.

a. $S = k \ln[\Omega(E)]$

Explain $\Omega(E)$

$\Omega(E)$ is the number of accessible states given an energy E .

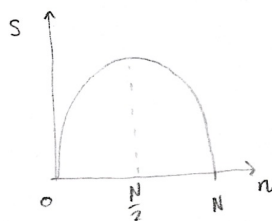
b. Write formula for $S(n)$ and sketch it

$n \rightarrow$ # of particles in upper state.

$E = 2\mu H n_{\uparrow}$ $N = n_{\uparrow} + n_{\downarrow}$

$\Omega(E) = \frac{N!}{n_{\uparrow}! (N - n_{\uparrow})!}$

$S(n) = k_B \ln[\Omega(n)] = k_B \ln \left[\frac{N!}{n_{\uparrow}! (N - n_{\uparrow})!} \right]$



c. Use Stirling's approximation for large n : $\ln n! = n \ln n - n$

$$\begin{aligned} S(n) &= k_B \left[\ln N! - \ln(n_{\uparrow}! (N - n_{\uparrow})!) \right] = k_B \ln N! - k_B \ln n_{\uparrow}! - k_B \ln (N - n_{\uparrow})! \\ &= k_B \left\{ (N \ln N - N) - (n_{\uparrow} \ln n_{\uparrow} - n_{\uparrow}) - [(N - n_{\uparrow}) \ln (N - n_{\uparrow}) - (N - n_{\uparrow})] \right\} \\ &= k_B \left\{ N \ln N - n_{\uparrow} \ln n_{\uparrow} - N \ln (N - n_{\uparrow}) + n_{\uparrow} \ln (N - n_{\uparrow}) - N + n_{\uparrow} + N - n_{\uparrow} \right\} \\ &= k_B \left\{ N [\ln N - \ln (N - n_{\uparrow})] - n_{\uparrow} [\ln n_{\uparrow} - \ln (N - n_{\uparrow})] \right\} \\ &= k_B \left[N \ln \left(\frac{N}{N - n_{\uparrow}} \right) - n_{\uparrow} \ln \left(\frac{n_{\uparrow}}{N - n_{\uparrow}} \right) \right] = k_B \left[N \ln \left(\frac{N}{N - n_{\uparrow}} \right) + n_{\uparrow} \ln \left(\frac{N - n_{\uparrow}}{n_{\uparrow}} \right) \right] \end{aligned}$$

Find max of $S(n)$.

$\frac{\partial S}{\partial n_{\uparrow}} = k_B \left[\frac{\partial}{\partial n_{\uparrow}} N \ln \left(\frac{N}{N - n_{\uparrow}} \right) + \frac{\partial}{\partial n_{\uparrow}} n_{\uparrow} \ln \left(\frac{N - n_{\uparrow}}{n_{\uparrow}} \right) \right]$

$= k_B N \cdot \frac{1}{N - n_{\uparrow}} + k_B \ln \left(\frac{N - n_{\uparrow}}{n_{\uparrow}} \right) + k_B n_{\uparrow} \left(\frac{-1}{n_{\uparrow}} - \frac{1}{N - n_{\uparrow}} \right) = \frac{k_B N}{N - n_{\uparrow}} + k_B \ln \left(\frac{N}{n_{\uparrow}} - 1 \right) - k_B + \frac{k_B n_{\uparrow}}{N - n_{\uparrow}}$

$= k_B \left[\frac{N - n_{\uparrow}}{N - n_{\uparrow}} - 1 + \ln \left(\frac{N}{n_{\uparrow}} - 1 \right) \right] = k_B \ln \left(\frac{N}{n_{\uparrow}} - 1 \right) = 0$

$\frac{N}{n_{\uparrow}} - 1 = 1$

$\frac{N}{n_{\uparrow}} = 2 \quad n_{\uparrow} = \frac{N}{2}$

Max S when $n_{\uparrow} = \frac{N}{2}$

d. Treat E as continuous. Show system can have a negative T .

$$\frac{\partial S}{\partial E} = \frac{1}{T}$$

$$S = k_B \left[N \ln \left(\frac{N}{N-n_u} \right) + n_u \ln \left(\frac{N-n_u}{n_u} \right) \right]$$

$$= k_B N \left[\ln \left(\frac{N}{N-n_u} \right) + \frac{n_u}{N} \ln \left(\frac{N}{n_u} - 1 \right) \right]$$

$$= k_B N \left[\ln \left(\frac{N}{N - \frac{E}{2\mu_H}} \right) + \frac{E}{2\mu_H N} \ln \left(\frac{N}{\frac{E}{2\mu_H}} - 1 \right) \right]$$

$$= k_B N \left[\ln \left(\frac{2\mu_H N}{2\mu_H N - E} \right) + \frac{E}{2\mu_H N} \ln \left(\frac{2\mu_H N}{E} - 1 \right) \right]$$

$$E = 2\mu_H n_u$$

$$n_u = \frac{E}{2\mu_H}$$

$$\frac{\partial S}{\partial E} = k_B N \left[\frac{-\partial}{\partial E} \ln(2\mu_H N - E) + \frac{E}{2\mu_H N} \frac{\partial}{\partial E} \ln \left(\frac{2\mu_H N}{E} - 1 \right) + \frac{1}{2\mu_H N} \ln \left(\frac{2\mu_H N}{E} - 1 \right) \right]$$

$$= k_B N \left[\frac{1}{2\mu_H N - E} + \frac{E}{2\mu_H N} \frac{1}{\frac{2\mu_H N}{E} - 1} \cdot \frac{-2\mu_H N}{E^2} + \frac{1}{2\mu_H N} \ln \left(\frac{2\mu_H N}{E} - 1 \right) \right]$$

$$= k_B N \left[\frac{1}{2\mu_H N - E} + \frac{-1}{2\mu_H N - E} + \frac{1}{2\mu_H N} \ln \left(\frac{2\mu_H N}{E} - 1 \right) \right] = \frac{k_B}{2\mu_H} \ln \left(\frac{2\mu_H N}{E} - 1 \right) = \frac{1}{T}$$

$$\frac{k_B}{2\mu_H} \ln \left(\frac{2\mu_H N}{E} - 1 \right) > 0 \quad \text{when}$$

$$\frac{2\mu_H N}{E} - 1 > 1 \Rightarrow \frac{2\mu_H N}{E} > 2$$

$$2\mu_H N > E$$

$$2\mu_H n_u$$

$$N > 2n_u$$

$$\frac{N}{2} > n_u$$

For $2\mu_H N > E$, T is negative, or for $\frac{N}{2} > n_u$.

e. Why is the negative temperature possible here but not for gas in box?

For a continuous system, adding energy increases the entropy. For this discrete two-level system, this is not the case. As we add energy, we increase the number of states in the upper level, hence reducing the number of states in the lower level. Once there are $\frac{N}{2}$ particles in the upper level, adding energy decreases the entropy, as there are less accessible states.

The maximum energy when N particles are in upper state actually has lowest entropy.