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1. Spreadsheet for plotting energy and specific heat of a system of N harmonic oscillators (Einstein Solid)
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1. Learning Outcomes

After studying this module, you shall be able to

- See the importance of Planck's constant in enumerating the number of allowed microstates in the light of Heisenberg uncertainty principle.
- Recognize the constraints under which micro canonical ensemble is defined and characterized by thermodynamic variables.
- Write the micro-canonical density distribution function.
- Clarify why a small amount of arbitrarily small uncertainty in energy ΔE around E is needed to count total number of allowed microscopic states.
- Calculate allowed number of microstates and hence entropy in an arbitrarily thin shell of a given microscopic ensemble for sample prototype models
 - Classical ideal gas
 - A two level system
 - A system of classical harmonic oscillators
 - Magnetization of a system of spin $\frac{1}{2}$ particles.

2. Introduction

In this module we will study the highly constrained ensemble the so called micro canonical ensemble, representing a system having constant energy E , constant number of particles N and constant volume V . It describes a system which is completely isolated system from its surroundings, a highly idealized situation seldom encountered in real situations. Within these constraints particles of the system can be in any one of the allowed microstates with equal a priori probability. Following the prescription described in module..... an effort is made to count the allowed total number of microstates which helps define the probability of each state followed by calculation of entropy which can then be used to calculate the thermodynamic properties of the system under study. But before embarking on this plan for micro-canonical ensemble we shall underline the importance of Planck's constant in the light of Heisenberg Uncertainty Principle in counting the microstates in the allowed phase space of the system under study.

3. Phase Space and Number of Microscopic States

As yet, till this point we have described the enumeration of microstates in terms of calculating the volume of the allowed phase space. This enumeration of microstates is possible through Heisenberg's Uncertainty Principle according to which phase space can be regarded as made up of elementary cells of the minimum volume h^d where d is the dimension of the phase space representing single particle quantum state. In the case of an N particle system with phase space having $6N$ dimensions, $d = 3N$.

4. Micro-canonical Ensemble Distribution Function

To define micro-canonical distribution function we must ponder on a crucial question, can we have an absolutely isolated system, because in actual systems, there is always some contact with the surroundings and system does not have a sharp value and it will have a width Δ around E . Hence system has a range of energy values $\left(E - \frac{1}{2}\Delta, E + \frac{1}{2}\Delta\right)$, where Δ is small compared to E . Doing this implies that a system has a large number of possible microstates in the phase space lying anywhere between a hyper-shell are equally apriori probable such that

$$E - \frac{1}{2}\Delta \leq H \leq E + \frac{1}{2}\Delta \quad (1)$$

This defines a region in phase space having volume

$$\omega = \int \Theta\left(E + \frac{1}{2}\Delta - H\right) \Theta\left(H - E + \frac{1}{2}\Delta\right) d^{3N}q d^{3N}p \quad (2)$$

Where Θ represents a unit step function defined by

$$\Theta(x) = \begin{cases} 1 & \text{if } x \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

The step functions sitting as integrand restrict the region of integration defined by equation (1). It is obvious that allowed phase space volume is a function of E, N, V and Δ .

Then a microcanonical ensemble is a collection of systems, for which probability distribution function $\rho(\mathbf{q}, \mathbf{p})$ in equilibrium is given by

$$\rho(\mathbf{q}, \mathbf{p}) = \begin{cases} \text{Constant for } E - \frac{1}{2}\Delta \leq H \leq E + \frac{1}{2}\Delta \\ 0 & \text{otherwise} \end{cases} \quad (4)$$

Now if $f(\mathbf{q}, \mathbf{p})$ is a physical quantity then the microcanonical ensemble average is given by

$$\langle f \rangle = \frac{\int \rho(\mathbf{q}, \mathbf{p}) f(\mathbf{q}, \mathbf{p}) d^{3N}q d^{3N}p}{\int \rho(\mathbf{q}, \mathbf{p}) d^{3N}q d^{3N}p} = \frac{\int f(\mathbf{q}, \mathbf{p}) d^{3N}q d^{3N}p}{\int d^{3N}q d^{3N}p} \quad (5)$$

5. Applications

Now we will look at some prototype applications of micro-canonical ensemble

5.1 A Two Level System

Let us begin with a simple two level system, i.e. a system which has only two states accessible, consisting of N non-interacting particles, Figure 1. The lower level is the ground state of the system with zero energy and the other level is the first excited state of the system with energy ϵ . Both the states are non-degenerate. The higher energy states are not available to the system, because they exceed the total energy available to the system. Let N_0 and N_1 be the number of particles in the ground state and first excited state respectively, such that $N = N_0 + N_1$.

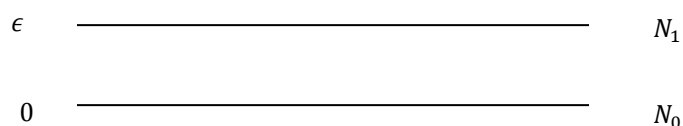


Figure 1 A two non-degenerate level system

The energy of the system is $E = N_1 \epsilon$. If we assume particles to be distinguishable then the number of microstates is the number of possible ways of choosing N_1 particles out of total N particles to fill the excited level which we call Ω and is given by:

$$\Omega = \binom{N}{N_1} = \frac{N!}{(N - N_1)! N_1!} \quad (6)$$

we are dealing with a thermodynamic system with large N and N_1 , we can use Stirling's approximation to calculate entropy S at a system at equilibrium. Boltzmann relation $S = k_B \ln \Omega$:

$$S = k_B [N \ln N - (N - N_1) \ln(N - N_1) - N_1 \ln N_1] \quad (7)$$

Noting that $N_1 = \frac{E}{\epsilon}$, equation (7) becomes

$$S = k_B \left[N \ln N - \left(N - \frac{E}{\epsilon}\right) \ln \left(N - \frac{E}{\epsilon}\right) - \frac{E}{\epsilon} \ln \frac{E}{\epsilon} \right] \quad (8)$$

Which can be simplified further as

$$S = k_B \left[\left(\frac{E}{\epsilon} - N \right) \ln \left(1 - \frac{E}{N\epsilon} \right) - \frac{E}{\epsilon} \ln \frac{E}{N\epsilon} \right] \quad (9)$$

Equation (9) provides us entropy for the system as a function of extensive variables E and N . Now we are ready to all other measurable thermodynamic quantities like temperature T , energy E and specific heat C_V .

Temperature can be obtained by using the relation $\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{N,V}$

$$\frac{1}{T} = \frac{k_B}{\epsilon} \left[\ln \left(1 - \frac{E}{N\epsilon} \right) + (E - N\epsilon) \left(\frac{N\epsilon}{N\epsilon - E} \right) \left(-\frac{1}{N\epsilon} \right) - \ln \frac{E}{N\epsilon} - E \frac{N\epsilon}{E} \frac{1}{N\epsilon} \right] \quad (10)$$

Or

$$\frac{1}{T} = \frac{k_B}{\epsilon} \left[\ln \left(1 - \frac{E}{N\epsilon} \right) - \ln \frac{E}{N\epsilon} \right] \quad (11)$$

Or

$$\frac{1}{T} = \frac{k_B}{\epsilon} \left[\ln \left(\frac{N\epsilon}{E} - 1 \right) \right] \quad (12)$$

Equation (12) also then gives expression for energy E as

$$E = \frac{N\epsilon}{1 + e^{\frac{\epsilon}{k_B T}}} \quad (13)$$

This effectively means

$$N_1 = \frac{N}{1 + e^{\frac{\epsilon}{k_B T}}} \quad (14)$$

The molar specific heat capacity, when $N = \text{Avogadro's number}$ can be obtained by recalling that $C_V = \left(\frac{\partial E}{\partial T} \right)_{N,V}$ which gives

$$C_V = k_B N \left(\frac{\epsilon}{k_B T} \right)^2 \frac{e^{\frac{\epsilon}{k_B T}}}{\left(e^{\frac{\epsilon}{k_B T}} + 1 \right)^2} \quad (15)$$

Let us look at some limiting cases:

Case I: $\frac{\epsilon}{k_B T} \gg 1$ (i.e. $T \rightarrow 0$)

According to equation (14), then denominator $(e^{\frac{\epsilon}{k_B T}} + 1)$ is very large and $N_1 \rightarrow 0$. This means that all particles are sitting in the ground state, total energy (equation (13)) $E = 0$ and $\Omega = 1$ and hence $S = 0$.

Case II: $\frac{\epsilon}{k_B T} \ll 1$ (i.e. $T \rightarrow \infty$)

According to equation (14), under this limit since $e^{\frac{\epsilon}{k_B T}} \rightarrow 1$, denominator becomes equal to 2 and hence $N_1 = \frac{N}{2}$ i.e. half the particles are in first excited state and half in ground state, energy of the two level system is $E = \frac{N\epsilon}{2}$ and hence entropy $S = k_B N \ln 2$

Let us look at the behavior of molar specific heat C_V , in both the limits (Case I and Case II) according to equation (15) C_V approaches zero and has maxima at $T = 0.42 \frac{\epsilon}{k_B}$ (or $\frac{\epsilon}{k_B T} = 2.38$) as shown in figure 2 below

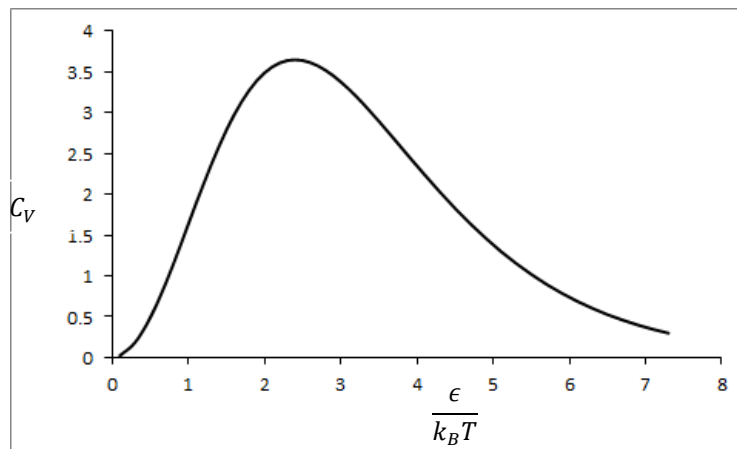


Figure 2 Molar specific heat capacity of a two level system (Schottky Anomaly)

Schottky anomaly found here is a characteristic feature of the systems having a pair of low lying energy levels with other levels of the system lying at a much higher level.

5.2 Classical Ideal Gas

In module VIII we discussed at length classical ideal gas from statistical mechanics route. Here we shall revisit this from the point of view definition of micro-canonical distribution function defined in equation (4). Accordingly the volume of the phase space accessible to the phase points in the micro canonical ensemble is ω :

$$\omega = \int \int' d^{3N}q d^{3N}p \quad (16)$$

Here prime on the integral sign indicates that the particles are fixed in a volume V and the total energy of the system, which in the case of ideal gas is kinetic energy, lies between the limits $E - \frac{1}{2}\Delta \leq \frac{p_i^2}{2m} \leq E + \frac{1}{2}\Delta$. Furthermore, since Hamiltonian is a function of p_i only the integration over the position co-ordinates can be performed yielding a factor of V^N . The remaining integral is the volume of a $3N$ dimensional shell enclosed by two hyperspheres of radii $\sqrt{[2m(E - \frac{1}{2}\Delta)]}$ and $\sqrt{[2m(E + \frac{1}{2}\Delta)]}$. For $\Delta \ll E$, it is thickness of the shell, $\Delta \left(\frac{m}{2E}\right)^{\frac{1}{2}}$, times surface area of the $3N$ dimensional hypersphere of radius $\sqrt{2mE}$. In module X, we had derived it for an n dimensional hypersphere and is

$$S_n = \frac{2\pi^{\frac{n}{2}}}{\left(\frac{n}{2} - 1\right)!} r^{n-1}$$

Thus volume of the desired $3N$ dimensional hyper-shell is

$$\Delta \left(\frac{m}{2E}\right)^{\frac{1}{2}} \frac{2\pi^{\frac{3N}{2}}}{\left(\frac{3N}{2} - 1\right)!} (2mE)^{\frac{3N-1}{2}}$$

Therefore, the phase space volume accessible to the representative points of the system is

$$\omega \cong \frac{\Delta}{E} V^N \frac{(2\pi mE)^{\frac{3N}{2}}}{\left(\frac{3N}{2} - 1\right)!} \quad (17)$$

Hence the number of microstates is

$$\Omega = \frac{\omega}{h^{3N}} = \frac{3N \Delta}{2 E} \frac{\left(\frac{2\pi mEV^{\frac{2}{3}}}{h^2}\right)^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!} \quad (18)$$

Therefore, entropy is given by using $S = k \ln \Omega$:

$$S = k_B N \left[\ln \left\{ V \left(\frac{2\pi m E}{h^2} \right)^{\frac{3}{2}} \right\} - \frac{3}{2} \ln \left(\frac{3N}{2} \right) + \frac{3}{2} + \frac{1}{N} \ln \left(\frac{3N \Delta}{2 E} \right) \right] \quad (19)$$

For large N , the last term in the expression is negligible hence

$$S = k_B N \left[\ln \left\{ V \left(\frac{2\pi m E}{h^2} \right)^{\frac{3}{2}} \right\} - \frac{3}{2} \ln \left(\frac{3N}{2} \right) + \frac{3}{2} \right] \quad (20)$$

This expression though expresses S as a function of E, V, N but is still not correct and needs to be corrected for indistinguishability, which led to Gibbs paradox. Once the expression is corrected by dividing Ω by $N!$, the other thermodynamic properties can be calculated (see module VIII).

5.3 A Collection of Linear Harmonic Oscillators

Here we are interested in a system of N harmonic oscillators of same frequency ω in micro-canonical ensemble with total energy E . The Hamiltonian of the system is given by

$$H = \sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 q_i^2 \right) \quad (21)$$

We shall look at this problem as a collection of classical oscillators and a collection of quantum mechanical oscillators and compare the two results later

5.3.1 Classical Approach:

Classically it amounts to finding the volume of the phase space ω within the hypershell of radii lying in the interval $E - \Delta \leq \sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 q_i^2 \right) \leq E$. This is $\omega = \Delta$ times the surface area of the volume of the phase space bounded by the surface $\sum_{i=1}^N \left(\frac{p_i^2}{2m} + \frac{1}{2} m \omega^2 q_i^2 \right) = E$, which is the derivative of the phase space bounded by the surface $\sum_{i=1}^N \left(\frac{p_i^2}{2mE} + \frac{q_i^2}{\frac{1}{2} m \omega^2 E} \right) = 1$. The volume of this $2N$ dimensional hypersphere can be obtained from the volume of a generalized sphere in n dimensional space bounded by the surface $\sum_{i=1}^d \frac{x_i^2}{a_i^2} = 1$ given by

$$V_d = \frac{\pi^{\frac{d}{2}}}{\frac{d}{2}!} \prod_{i=1}^d a_i \quad (22)$$

Using equation (22) we get

$$V_{2N} = \frac{\pi^N}{N!} (2mE)^{\frac{N}{2}} \left(\frac{2E}{m\omega^2}\right)^{\frac{N}{2}} = \frac{1}{N!} \left(\frac{2\pi E}{\omega}\right)^N \quad (23)$$

Therefore, the surface area can be obtained by taking derivative of (23) with respect to E and one gets,

$$S_{2N} = \frac{dV}{dE} = \frac{1}{N!} N \left(\frac{2\pi}{\omega}\right)^N E^{(N-1)} = \frac{1}{N!} \left(\frac{2\pi E}{\omega}\right)^N \frac{N}{E} \quad (24)$$

So the volume of the hypershell of phase space with allowed representative points is given by

$$\omega = \frac{1}{N!} \left(\frac{2\pi E}{\omega}\right)^N \frac{N\Delta}{E} \quad (25)$$

The number of microstates $\Omega = \frac{\omega}{h^N}$ then is given by

$$\Omega = \frac{1}{N!} \left(\frac{2\pi E}{h\omega}\right)^N \frac{N\Delta}{E} \quad (26)$$

Entropy of this collection of N linear harmonic oscillators is then given by

$$S = Nk_B \left[\ln \left(\frac{2\pi E}{h\omega}\right) - \ln N + 1 + \frac{1}{N} \ln \frac{N\Delta}{E} \right] \quad (27)$$

The last term in (27) can be neglected since it has a very small contribution compared other terms.

$$S = Nk_B \left[\ln \left(\frac{2\pi E}{Nh\omega}\right) + 1 \right] \quad (28)$$

Now we are ready to calculate other thermodynamic quantities such as Temperature and Helmholtz free energy.

Temperature is given by

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{V,N} = Nk_B \left[\frac{Nh\omega}{2\pi E} \frac{2\pi}{Nh\omega} \right] = \frac{Nk_B}{E} \quad (29)$$

Also we get

$$E = Nk_B T \quad (30)$$

Helmholtz free energy can now be obtained using the relation $F = E - TS$

$$F = -T Nk_B \left[\ln \left(\frac{2\pi E}{Nh\omega} \right) \right] = Nk_B T \left[\ln \left(\frac{h\omega}{2\pi k_B T} \right) \right] \quad (31)$$

5.3.1 Quantum Approach:

Quantum mechanically, each oscillator has an energy eigen value given by well known relation

$$\epsilon_i = \left(n_i + \frac{1}{2} \right) \hbar \omega \quad (32)$$

Where n_i is a an integer ≥ 0 . The total energy of the system is then given by

$$E = \left(n + \frac{N}{2} \right) \hbar \omega \quad (33)$$

Where $n = n_1 + n_2 + n_3 \dots \dots \dots + n_N$ is a non-negative integer.

Now to calculate the number of microstates corresponding to this total energy. Let us note that this amounts to distributing n packets of energy in N boxes, where each box can contain any number of packets including possibility of zero packets. If we wish to create N boxes in a box we require $N-1$ partitions, so to count the number of possible ways to distribute n energy packets in N boxes is equivalent to arranging a total of n packets and $N-1$ partitions together, i.e. permuting $n+N-1$ out of which n packets among them are indistinguishable and $N-1$ partitions among them are indistinguishable.

Therefore,

$$\Omega = \frac{(n + N - 1)!}{n! (N - 1)!} \quad (34)$$

The entropy of the system after using stirlings approximation is then given by

$$S = k_B \ln \Omega = k_B [(n + N - 1) \ln(n + N - 1) - n \ln n - (N - 1) \ln(N - 1)] \quad (35)$$

Since in thermodynamic limit, $N \gg 1$, $N - 1 \cong N$ and $n = \left(\frac{E}{\hbar\omega} - \frac{N}{2}\right)$, equation (35) becomes

$$S = k_B \left[\left(\frac{E}{\hbar\omega} + \frac{N}{2}\right) \ln \left(\frac{E}{\hbar\omega} + \frac{N}{2}\right) - \left(\frac{E}{\hbar\omega} - \frac{N}{2}\right) \ln \left(\frac{E}{\hbar\omega} - \frac{N}{2}\right) - N \ln N \right] \quad (36)$$

Or

$$S = Nk_B \left[\left(\frac{E}{N\hbar\omega} + \frac{1}{2}\right) \ln \left(\frac{E}{N\hbar\omega} + \frac{1}{2}\right) - \left(\frac{E}{N\hbar\omega} - \frac{1}{2}\right) \ln \left(\frac{E}{N\hbar\omega} - \frac{1}{2}\right) \right] \quad (37)$$

Now we are ready to derive all thermodynamic relations

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{N,V} = \frac{k_B}{\hbar\omega} \left(\ln \left(\frac{E}{N\hbar\omega} + \frac{1}{2}\right) - \ln \left(\frac{E}{N\hbar\omega} - \frac{1}{2}\right) \right) \quad (38)$$

Or

$$\frac{\left(\frac{E}{N\hbar\omega} + \frac{1}{2}\right)}{\left(\frac{E}{N\hbar\omega} - \frac{1}{2}\right)} = e^{\frac{\hbar\omega}{k_B T}} \quad (39)$$

Or

$$E = N \hbar\omega \left\{ \frac{1}{2} + \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} \right\} \quad (40)$$

It is interesting to ask what happens to equation (40), a quantum mechanical result in the classical limit i.e. when $\frac{\hbar\omega}{k_B T} \ll 1$.

$$E \approx N \left\{ \frac{\hbar\omega}{2} + \hbar\omega \frac{k_B T}{\hbar\omega} \right\} \approx N k_B T \quad (41)$$

Same result as the classical result (30).

Furthermore, specific heat at constant volume $C_V = \left(\frac{\partial E}{\partial T} \right)_{N,V}$ can be obtained as

$$C_V = N k_B \left(\frac{\hbar\omega}{k_B T} \right)^2 \frac{e^{\frac{\hbar\omega}{k_B T}}}{\left(e^{\frac{\hbar\omega}{k_B T}} - 1 \right)^2} \quad (42)$$

In the classical limit, it becomes

$$C_V \approx N k_B \left(\frac{\hbar\omega}{k_B T} \right)^2 \frac{1}{\left(\frac{\hbar\omega}{k_B T} \right)^2} = N k_B \quad (43)$$

Similarly Helmholtz free energy in quantum and classical limits can be obtained.

Figures 3 and 4 below show respectively the plot of $\frac{E}{N\hbar\omega}$ and C_V against $\frac{k_B T}{\hbar\omega}$.

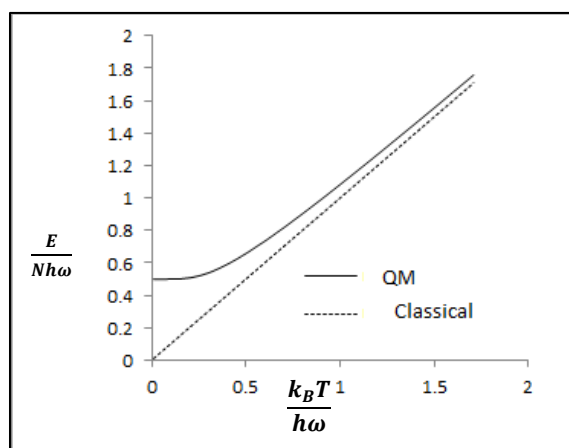


Figure 3 $\frac{E}{N\hbar\omega}$ versus $\frac{k_B T}{\hbar\omega}$

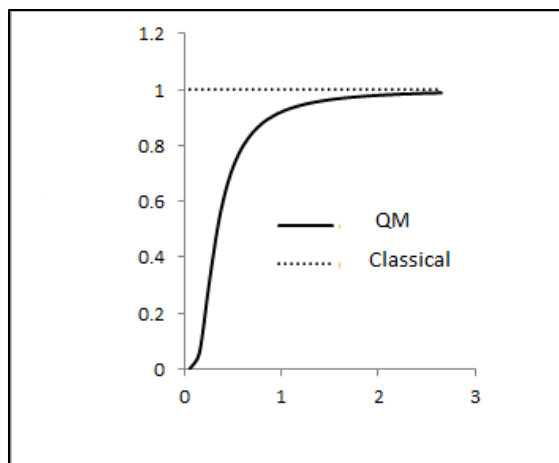


Figure 4 $\frac{C_V}{Nk_B}$ versus $\frac{k_B T}{\hbar\omega}$ for a collection of N Harmonic Oscillators

This example actually represents model of an Einstein solid made of N uncoupled quantum oscillators of same frequency.

5.4 A System of Spin $\frac{1}{2}$ Particles

We now consider an isolated system of N particles of spin $\frac{1}{2}$, i.e. $\vec{\sigma}_i = \frac{1}{2} \hbar \hat{z} = \sigma_i^z \hat{z}$. Each particle in the system, therefore has a magnetic moment $\mu \vec{\sigma}$. Placed in a magnetic field \vec{H} such a particle has only two orientations, spin up (\uparrow) or spin down (\downarrow) with respect to the magnetic field. Let the magnetic field be in the direction of Z -axis.

The Hamiltonian for such a system is given by

$$\mathcal{H} = - \sum_{i=1}^N \mu \vec{\sigma}_i \cdot \vec{H} = -\mu H \sum_{i=1}^N \sigma_i^z \quad (44)$$

The Hamiltonian does not have a term for the motion of the particles except interaction with the magnetic field. System has number of particles N and total magnetic moment M as extensive parameters, Volume has no role to play in this situation.

Suppose that at equilibrium system has N_+ particles with spin up and N_- particles with spin down, such that

$$N = N_+ + N_- \quad (45)$$

The net magnetic moment of the system is then

$$M = \mu(N_+ - N_-) \quad (46)$$

Solving (45) and (46) for N_+ and N_- , we have

$$N_{\pm} = \frac{N}{2} \left(1 \pm \frac{M}{\mu N} \right) \quad (47)$$

So to count the number of microstates it is merely a matter of selecting N_+ number of particles out of N particles and is given by

$$\Omega(M, N) = \frac{N!}{N_+! N_-!} \quad (48)$$

Entropy can then be obtained from Boltzmann relationship $S = k_B \ln \Omega(M, N)$ as

$$S(M, N) = k_B (\ln N! - \ln N_+! - \ln N_-!) \quad (49)$$

In thermodynamic limit using Stirlings Formula and (47), we have

$$S(M, N) = k_B \left(N \ln N - \frac{N}{2} \left(1 + \frac{M}{\mu N} \right) \ln \frac{N}{2} \left(1 + \frac{M}{\mu N} \right) - \frac{N}{2} \left(1 - \frac{M}{\mu N} \right) \ln \frac{N}{2} \left(1 - \frac{M}{\mu N} \right) \right) \quad (50)$$

Or

$$S(M, N) = N k_B \left(\ln 2 - \frac{1}{2} \left(1 + \frac{M}{\mu N} \right) \ln \left(1 + \frac{M}{\mu N} \right) - \frac{1}{2} \left(1 - \frac{M}{\mu N} \right) \ln \left(1 - \frac{M}{\mu N} \right) \right) \quad (51)$$

Equation (51) is the entropy of the system in terms of extensive variables M and N .

Knowing that $\left(\frac{\partial S}{\partial M} \right)_{E, V, N} = -\frac{H}{T}$

We have

$$-\frac{H}{T} = \frac{k_B}{2\mu} \ln \frac{\mu N - M}{\mu N + M} \quad (52)$$

Which can be further simplified to give the expression for magnetic moment

$$M = \mu N \frac{\left(e^{\frac{\mu H}{k_B T}} - e^{-\frac{\mu H}{k_B T}} \right)}{\left(e^{\frac{\mu H}{k_B T}} + e^{-\frac{\mu H}{k_B T}} \right)} = \mu N \tanh \frac{\mu H}{k_B T} \quad (53)$$

This is the equation of state of a system with N particles of spin $\frac{1}{2}$.

Before we end, it will be interesting to explore $\ln \Omega(M, N)$ using (51). noting that for $0 < x < 1$, $\ln(1 \pm x) \cong \pm x - \frac{x^2}{2} \pm \frac{x^3}{3} - \dots$ we have

$$\ln \Omega(M, N) = N \left(\ln 2 - \frac{1}{2} \left(\frac{M}{\mu N} \right)^2 \right) \quad (54)$$

We have

$$\Omega(M, N) = e^{(N \ln 2)} e^{-\frac{1}{2N} \left(\frac{M}{\mu} \right)^2} \approx e^{-\frac{1}{2N} \left(\frac{M}{\mu} \right)^2} \quad (55)$$

This is a Gaussian distribution with a spread of \sqrt{N} as shown in figure

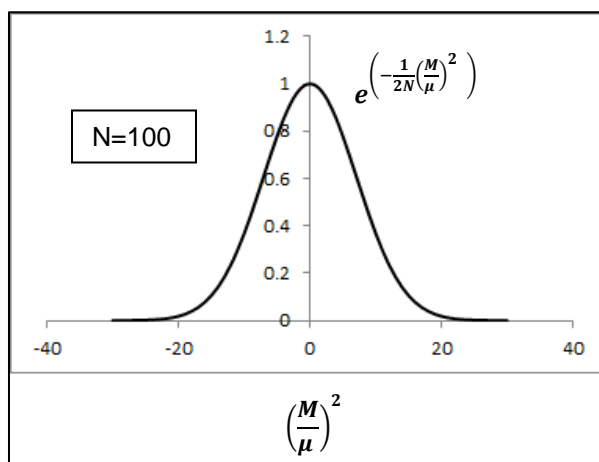


Figure 5 Gaussian distribution equation (55)

5. Summary

In this module we have learnt

- That micro canonical ensemble corresponds to a collection of exact replicas of completely isolated system with $E = \text{constant}$, $N = \text{constant}$ and $V = \text{constant}$.

- That micro-canonical distribution function is defined as

$$\rho(\mathbf{q}, \mathbf{p}) = \begin{cases} \text{Constant for } E - \frac{1}{2}\Delta \leq H \leq E + \frac{1}{2}\Delta \\ 0 & \text{otherwise} \end{cases}$$

Where $E - \frac{1}{2}\Delta \leq H \leq E + \frac{1}{2}\Delta$ is a thin shell of energy with width $\Delta \ll E$

- the microcanonical ensemble average is given by

$$\langle f \rangle = \frac{\int \rho(\mathbf{q}, \mathbf{p}) f(\mathbf{p}, \mathbf{q}) d^{3N}q d^{3N}p}{\int \rho(\mathbf{q}, \mathbf{p}) d^{3N}q d^{3N}p} = \frac{\int f(\mathbf{p}, \mathbf{q}) d^{3N}q d^{3N}p}{\int d^{3N}q d^{3N}p}$$

- that micro canonical ensemble can be applied to study some interesting prototype problems and following problems were studied to calculate the entropy and other thermodynamic properties

- A Two Level System
- Classical Ideal Gas
- A System of Linear Classical Harmonic Oscillators
- A system of Spin $\frac{1}{2}$ Particles

- That a two level system shows Schotkky anomaly in its specific heat. Two level system shows following limiting behaviour

Case I: $\frac{\epsilon}{k_B T} \gg 1$ (i.e. $T \rightarrow 0$) all the particles sit in the ground state, total energy $E = 0$ and $\Omega = 1$ and hence $S = 0$.

Case II: $\frac{\epsilon}{k_B T} \ll 1$ (i.e. $T \rightarrow \infty$). half the particles are in first excited state and half in ground state, energy of the two level system is $E = \frac{N\epsilon}{2}$ and hence entropy $S = k_B N \ln 2$

- That classical ideal gas can be studied using micro-canonical ensemble. The calculated entropy shows gibbs paradox, which needs correction for indistinguishability of particles
- That collection of N harmonic oscillators can be looked at classically as well as quantum mechanically with following results for entropy and various other thermodynamic quantities.

Thermodynamic Properties	
Collection of N Linear Classical H.O.	Collection of N Linear Quantum H.O.
$S = Nk_B \left[\ln \left(\frac{2\pi E}{Nh\omega} \right) + 1 \right]$	$S = Nk_B \left[\left(\frac{E}{N\hbar\omega} + \frac{1}{2} \right) \ln \left(\frac{E}{N\hbar\omega} + \frac{1}{2} \right) - \left(\frac{E}{N\hbar\omega} - \frac{1}{2} \right) \ln \left(\frac{E}{N\hbar\omega} - \frac{1}{2} \right) \right]$

Thermodynamic Properties	
Collection of N Linear Classical H.O.	Collection of N Linear Quantum H.O.
$E = Nk_B T$	$E = N \hbar \omega \left\{ \frac{1}{2} + \frac{1}{e^{\frac{\hbar \omega}{k_B T}} - 1} \right\}$
$C_V = Nk_B$	$C_V = Nk_B \left(\frac{\hbar \omega}{k_B T} \right)^2 \frac{e^{\frac{\hbar \omega}{k_B T}}}{\left(e^{\frac{\hbar \omega}{k_B T}} - 1 \right)^2}$

Quantum mechanical results approach classical results in the so called classical with limit, $\frac{\hbar \omega}{k_B T} \ll 1$.

- That a system of N particles with spin $\frac{1}{2}$ has a new extensive variable with following equation of state

$$M = \mu N \tanh \frac{\mu H}{k_B T}$$

- That a system of N particles with spin $\frac{1}{2}$ has a Gaussian density distribution with a spread \sqrt{N}

$$\Omega(M, N) \approx e^{\left(-\frac{1}{2N} \left(\frac{M}{\mu} \right)^2 \right)}$$

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Appendices:

1. [Spreadsheet for plotting energy and specific heat of a system of N harmonic oscillators \(Einstein Solid\)](#)
2. [Spreadsheet for probability distribution function for a system of N particles with spin half in a magnetic field \(gaussian distribution\)](#)