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Defining 'energy' in micro canonical ensemble

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Abstract

The micro canonical ensemble (MCE) represents an isolated system having fixed energy. The nature of energy in MCE is always a subject of discussion. In this paper we are distinguishing the energy possessed by the system and the energy offered by the system for measurement in MCE. This we hope will help the learners of statistical mechanics to have a more understanding of MCE.

Keywords: Microcanonical ensemble, Internal energy and quantum harmonic oscillator

1. Introduction

In micro canonical ensemble (MCE) we have energy (E), volume(V) and number of particles(N) as the constants of the system. But 'What is E ?' or on what factors E will depend, whether E is a function of temperature etc are the questions that came to our mind when we learn statistical mechanics. To answer all these questions we consider five examples in MCE and is trying to answer the questions raised above. The examples are N

1. Non relativistic free particles.
2. Relativistic mass less particles.
3. Quantum harmonic oscillators.

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4. Discrete energy systems.
5. Spin half particles in a magnetic field.

From the recipe of thermodynamics in MCE we know that temperature T is related to

entropy S by the equation

$$\frac{1}{T} = (\frac{\partial S}{\partial E})_{V,N} \tag{1}$$

This equation defines temperature as well the macroscopic energy. Fixing 'E' we get the number of micro states Ω and from entropy we get temperature using equation (1). In text books [1, 2, 3, 4, 5] we use the same notation to represent the energy of the system of particles and the energy we measure, which creates the confusion. Actually the input energy is temperature independent and the output energy is a function of temperature as indicated by the Equation (1). To avoid misinterpretation we will change E to **E** after the use of equation (1) which gives the output. In the next section we will take systems with classical, discrete and quantum energies and study five examples to demonstrate the differences between input and output energies.

2. Some case studies

2.1. Non relativistic ideal gas

Taking the energy of a particle as $\varepsilon = \frac{p^2}{2m}$ we get the total number of micro states for N particles as [1],

$$\Omega = \left(\frac{V}{h^3}\right)^N \frac{(2\pi mE)^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!N!} \tag{2}$$

where h is the Planck's constant. Using Boltzmann equation S = k ln Ω we get

$$S = k\ln\left[\left(\frac{V}{h^3}\right)^N \frac{(2\pi m E)^{\frac{3N}{2}}}{\left(\frac{3N}{2}\right)!N!}\right]$$

(3)

Substituting for entropy in Eq (1), we get the output energy as

$$\boldsymbol{E} = E = \frac{3}{2}NkT \tag{4}$$

2.2. Relativistic mass less particles

For a relativistic mass less particle the single particle energy is given by

$$\varepsilon = pc$$

The number of microstates will be [2]

$$\Omega = \frac{V^N}{(3N)!N!}\left(\frac{8\pi E^3}{c^3}\right)^N \frac{1}{h^{3N}}$$

(5)

and entropy is

$$S = k\ln\left[\frac{V^N}{(3N)!N!}\left(\frac{8\pi E^3}{c^3}\right)^N \frac{1}{h^{3N}}\right]$$

(6)

Substituting in Eq (1) we get the output energy as

$$\boldsymbol{E} = E = 3NkT \tag{7}$$

2.3 Quantum harmonic oscillator

In the case of systems with quantum origin (spin systems) the total number of micro states can be calculated by the equation

$$\Omega = \frac{(n_i + g_i - 1)!}{n_i!(g_i - 1)!}$$

where n_i is the number of particles per state and g_i is the available degeneracy's. Consider N localized non interacting one dimensional harmonic oscillator with energy $\hbar\omega$, where ω is the angular frequency.

Then $E_1 = \left(n_1 + \frac{1}{2}\right)\hbar\omega$, $E_2 = \left(n_2 + \frac{1}{2}\right)\hbar\omega$, and so on $E_n = \left(n_n + \frac{1}{2}\right)\hbar\omega$. Total energy

$$E = \left(M + \frac{N}{2}\right)\hbar\omega \tag{8}$$

where $M = n_1 + n_2 + \dots\dots + n_n$ with $M = \frac{E}{\hbar\omega} - \frac{N}{2}$. In this case we have to arrange N quantum harmonic oscillators in M states with $M = n_i$ and $N = g_i$. So

$$\Omega = \frac{(M + N - 1)!}{M!(N - 1)!} \tag{9}$$

Simplifying using the Stirlings approximation we get

$$S = k \ln \left[\left[\frac{E}{\hbar\omega} + \frac{N}{2}\right] \ln\left[\frac{E}{\hbar\omega} + \frac{N}{2}\right] - \left[\frac{E}{\hbar\omega} - \frac{N}{2}\right] \ln \left[\frac{E}{\hbar\omega} - \frac{N}{2}\right] - N \ln N\right] \quad (10)$$

and we get energy as

$$\boldsymbol{E} = \frac{N\hbar\omega}{2} + \frac{N\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1} \quad (11)$$

2.4. N particles with energy 0 and energy ε.

Let N_1 particles have energy 0 and N_2 particles have energy ε. Then input energy

$$E = N_1 * 0 + N_2 * \varepsilon$$

Using

$$\Omega = \frac{N!}{N_1 !N_2 !}$$

we get

$$S = k \left[\mathrm{N} \ln N - \left(N - \frac{E}{\varepsilon}\right) \ln\left(N - \frac{E}{\varepsilon}\right) - \left(\frac{E}{\varepsilon}\right) \ln\left(\frac{E}{\varepsilon}\right)\right] \quad (12)$$

and

$$\boldsymbol{E} = \frac{N\varepsilon}{e^{\frac{\varepsilon}{kT}} + 1} \quad (13)$$

2.5. N non interacting spin 1/2 particles in an external magnetic field H

Here $E = -\mu_0 H \sum_{i=1}^{N} \sigma_i$ where $\sigma_i = \pm 1$ and μ_0 is the free space permeability. Substituting the above energy we get

$$E = -\mu_0 H N_1 + \mu_0 H N_2$$

and

$$E = -N\mu_0 H \tanh(\beta\mu_0 H)$$

where $\beta = \frac{1}{kT}$

3. Results and discussions

Our results are given in the Table below.

No.	System	E	E
1	Non relativistic free particles	$\sum_{i=1}^{3N} \frac{p_i^2}{2m}$	$\frac{3}{2}NkT$
2	Relativistic mass less particles	$\sum_{i=1}^{3N} p_i c$	$3NkT$
3	Quantum harmonic oscillators	$\left(M + \frac{N}{2}\right)\hbar\omega$	$\frac{N\hbar\omega}{2} + \frac{N\hbar\omega}{e^{\frac{\hbar\omega}{kT}} - 1}$
4	Discrete energy systems	$N_2\varepsilon$	$\frac{N\varepsilon}{e^{\frac{\varepsilon}{kT}} + 1}$
5	Particles in a magnetic field	$-\mu_0 H N_1 + \mu_0 H N_2$	$-N\mu_0 H \tanh(\beta\mu_0 H)$

We can see that the input energy E is always independent of temperature. If it is a function of temperature, then there is no statistical mechanics. Output energy **E** depends on the system parameters like $\hbar\omega$, ε, $\mu_0 H$ etc and in classical cases it will always be a function of temperature, which agrees with equipartition theorem [2].

4. Conclusions

In this paper we with the help of some examples make a clear distinction between the input and output energies in MCE. We had shown that the input energy is always independent of temperature and the output energy will be functions of temperature and input energy parameters.

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