PHYS4006: Thermal and Statistical Physics

Lecture Notes
Part - 4 (Unit - IV)

Two Level System & Negative Temperature

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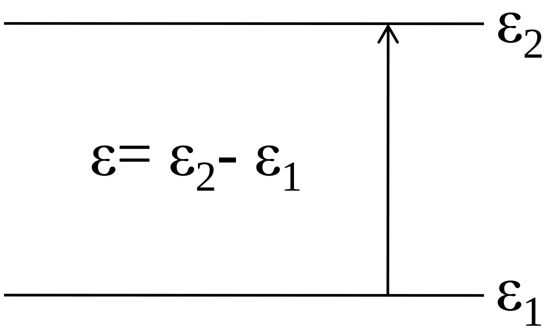
Two level energy system

- Consider a system having two non-degenerate microstates with energies ε_1 and ε_2. The energy difference between the levels is $\varepsilon = \varepsilon_2 - \varepsilon_1$



Let us assume that the system is in

thermal equilibrium at temperature T.

So, the partition function of the system is –

$$Z = \exp\left(-\frac{\varepsilon_1}{kT}\right) + \exp\left(-\frac{\varepsilon_2}{kT}\right) \quad ....(1)$$

The probability of occupancy of these states is given by -

$$P_1 = \frac{\exp\left(-\frac{\varepsilon_1}{kT}\right)}{Z} = \frac{\exp\left(-\frac{\varepsilon_1}{kT}\right)}{\exp\left(-\frac{\varepsilon_1}{kT}\right) + \exp\left(-\frac{\varepsilon_2}{kT}\right)} = \frac{1}{1 + \exp\left(-\frac{\varepsilon_2 - \varepsilon_1}{kT}\right)}$$

$$P_2 = \frac{\exp\left(-\frac{\varepsilon_2}{kT}\right)}{Z} = \frac{\exp\left(-\frac{\varepsilon_2}{kT}\right)}{\exp\left(-\frac{\varepsilon_1}{kT}\right) + \exp\left(-\frac{\varepsilon_2}{kT}\right)} = \frac{\exp\left(-\frac{\varepsilon_2 - \varepsilon_1}{kT}\right)}{1 + \exp\left(-\frac{\varepsilon_2 - \varepsilon_1}{kT}\right)}$$

or, $P_1 = \dfrac{1}{1 + \exp\left(-\frac{\theta}{T}\right)}$ ......(2) and $P_2 = \dfrac{\exp\left(-\frac{\theta}{T}\right)}{1 + \exp\left(-\frac{\theta}{T}\right)}$ ....(3)

where $\theta = \dfrac{\varepsilon_2 - \varepsilon_1}{k}$

From (2) and (3), we can see that P_1 and P_2 depends on T.

Thus, if T=0, P_1=1 and P_2=0 (*System is in ground state*)

When $T \ll \theta$, i.e. $kT \ll \varepsilon$ then P_2 is negligible and it begins to increase when temperature is increased.

- Consider a paramagnetic substance having N magnetic atoms per unit volume placed in an external magnetic field B. Assume that each atoms has spin ½ and an intrinsic magnetic moment μ_B. Let us suppose that the energy levels are non-degenerate, i.e. there is only one state in each level. As we know that the magnetic energy of an atom in an external field is - μ_B.B cosθ.

- The energy in the lower state (in which μ_B is parallel to the magnetic field B) is $\varepsilon_1 = -\mu_B.B$

- The energy of the higher state (in which μ_B is anti-parallel to the magnetic field B) is $\varepsilon_1 = \mu_B.B$

Thus, if the system is in thermal equilibrium at temperature T, then the partition function of the system can be written as -

$$Z = \exp\left(\frac{\mu_B B}{kT}\right) + \exp\left(-\frac{\mu_B B}{kT}\right) = 2\cosh\left(\frac{\mu_B B}{kT}\right) \quad ....(4)$$

If N_1 and N_2 are the number of atoms whose moments are parallel and anti-parallel to B, respectively then

$$N_1 = \frac{N}{Z}\exp\left(\frac{\mu_B B}{kT}\right) \quad ....(5) \qquad N_2 = \frac{N}{Z}\exp\left(\frac{-\mu_B B}{kT}\right) \quad ....(6)$$

Where $N=(N_1+N_2)$ denotes the total number of atoms.

The excess of atoms aligned parallel to B over those aligned anti-parallel to B is given by –

$$N_2 - N_1 = \frac{N}{Z}\left[\exp\left(\frac{\mu_B B}{kT}\right) - \exp\left(\frac{-\mu_B B}{kT}\right)\right] = \frac{2N}{Z}\sinh\left(\frac{\mu_B B}{kT}\right)$$

Putting the value of Z from (4), we get

$$N_2 - N_1 = N\tanh\left(\frac{\mu_B B}{kT}\right) \quad ....(7)$$

The net magnetic moment of the system is therefore,

$$M = \mu_B\left(N_2 - N_1\right) = N\mu_B\tanh\left(\frac{\mu_B B}{kT}\right) \quad ....(8)$$

For weak field and high temperatures, $\mu_B B << kT$, then

$$M = N\mu_B\left(\frac{\mu_B B}{kT}\right) = \frac{N\mu_B^2\mu_0 H}{kT} \quad ....(9) \quad \{\because B = \mu_0 H\}$$

and, Magnetic susceptibility is given by

$$\chi = \frac{M}{H} = \frac{N\mu_B^2\mu_0}{kT} \quad ....(10)$$

or, $\chi = \dfrac{C}{T}$ $\quad$ $where\ C = \dfrac{N\mu_B^2\mu_0}{k}$ (Curie constant)

Also, we know $M_{sat} = N\mu_B$ then from (8)

$$\frac{M}{M_{sat}} = \tanh\left(\frac{\mu_B B}{kT}\right) \quad ....(11)$$

Negative Temperature

- Let us consider a freely moving molecule of a perfect gas or a harmonic oscillator characterized by an infinite number of energy levels.

- As the temperature of the system is increased, more molecules will be raised to higher energy states thereby making the system more energetic and thus greater disorder.

- Thus, entropy increases as the energy increases. It means (dU/dS) will always be positive, i.e. positive temperature states.

However, let us proceed again by taking the previous example of paramagnetic atoms where occupation number of the two level system is given by –

$$N_1 = \frac{N}{Z}\exp\left(\frac{-\varepsilon_1}{kT}\right) \quad \text{and} \quad N_2 = \frac{N}{Z}\exp\left(\frac{-\varepsilon_2}{kT}\right)$$

where $N=(N_1+N_2)$ denotes the total number of atoms.

or,

$$\frac{N_1}{N_2} = \exp\left(\frac{\varepsilon_2 - \varepsilon_1}{kT}\right) \quad ....(12)$$

$$T = \frac{1}{k}\left(\frac{\varepsilon_2 - \varepsilon_1}{\ln N_1 - \ln N_2}\right) \quad ....(13)$$

Since, $\varepsilon_2 > \varepsilon_1 \rightarrow$ T will be positive (if $N_1 > N_2$).

Now, on reversing the direction of magnetic field, the dipoles oriented parallel to the field and having energy ε_1 will be oriented anti-parallel to the field and have a higher energy.

But, the dipoles originally anti-parallel to the field and having energy ε_2 will now be oriented parallel to the field and have a lower energy.

Let the average occupation numbers of the new lower and higher energy states be N'_1 and N'_2, respectively. Therefore, $N'_2=N_1$ and $N'_2>N'_1$. This is referred as ***'population inversion'***.

Now,

$$T' = \frac{1}{k}\left(\frac{\varepsilon_2 - \varepsilon_1}{\ln N_1' - \ln N_2'}\right) \quad ....(14)$$

Since, $N'_2>N'_1$, this state will correspond to **negative temperature**.

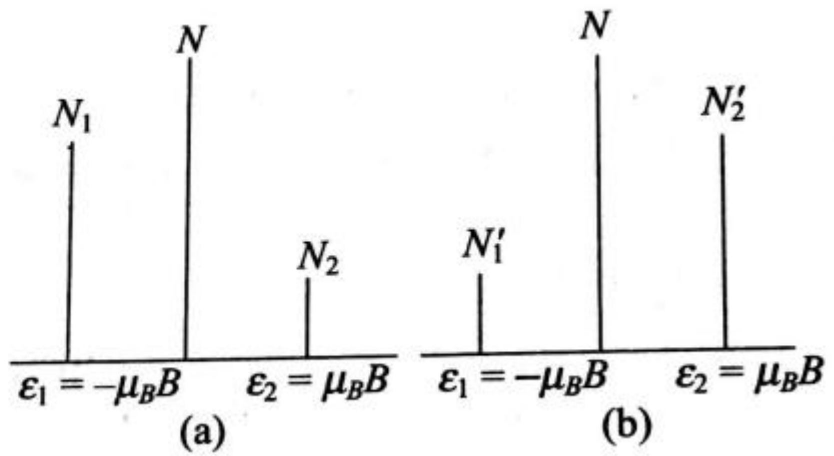


Figure: (a) in thermal equilibrium, $N_1 > N_2$; (b) case of population inversion, $N_2 > N_1$. Vertical lines signifies the level of occupancy of a state. [Garg, Bansal and Ghosh]

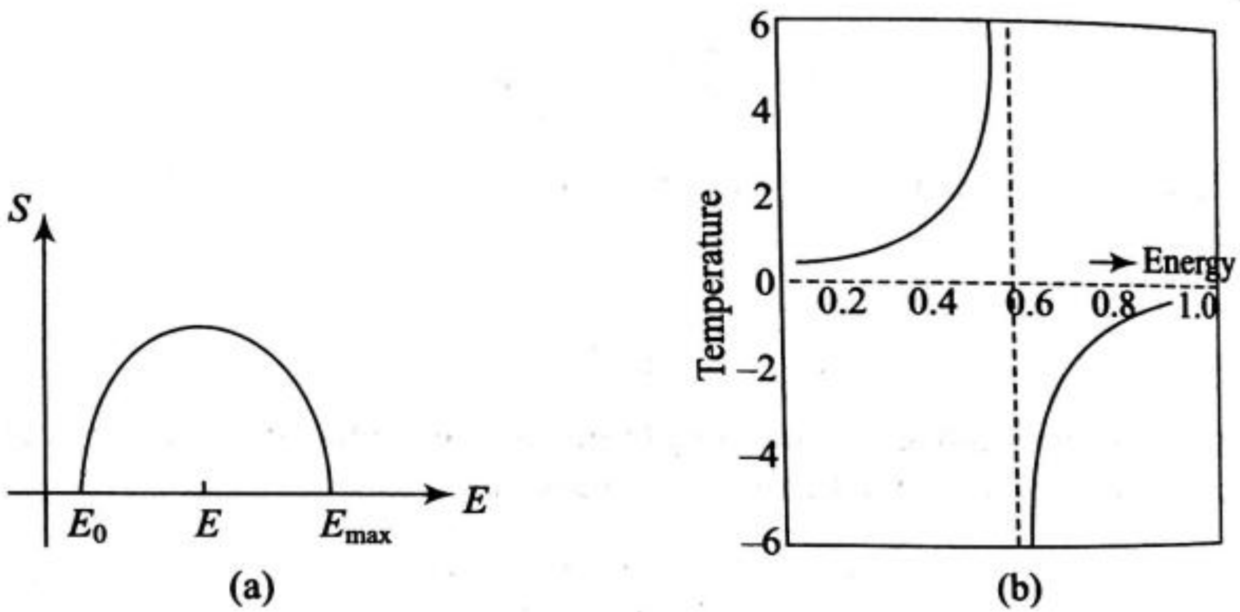


Figure: (a) plot of entropy as a function of internal energy for a two level system, $\varepsilon_1=0$ and $\varepsilon_2=\varepsilon$ (b) plot of temperature as a function of internal energy. [Garg, Bansal and Ghosh]

1. From eq^n. (2), it can be seen that for $T=0$, $P_1 \approx 1$, i.e. all the states will lie in the lower energy state $\varepsilon_1=0$; $N_1=N$ and $N_2=0$. This is a state of minimum disorder and corresponds to $S=0$. Internal energy of the system will also be zero.

2. As T increases, the occupancy in the higher level begins to takes place. As $T \rightarrow \infty$, $P_1=P_2=1/2$, i.e. $N_1=N_2=1/2$ and internal energy will be $N\varepsilon/2$. This state will correspond to maximum disorder and maximum entropy.

3. If more atoms tend to occupy the higher energy states such that $N_2>N_1$, i.e. population inversion has achieved. In a case, if $N_2=N$ then internal energy will be $N\varepsilon$. This corresponds to state of minimum disorder and zero entropy. Eq^n. (13) gives the negative temperature. It gives the state of ***negative temperature***.

References: Further Readings

1. *Statistical Mechanics* by R.K. Pathria

2. *Thermal Physics (Kinetic theory, Thermodynamics and Statistical Mechanics)* by S.C. Garg, R.M. Bansal and C.K. Ghosh

3. *Elementary Statistical Mechanics* by Gupta & Kumar

4. *Statistical Mechanics* by K. Huang

5. *Statistical Mechanics* by B.K. Agrawal and M. Eisner

Thank You

For any questions/doubts/suggestions and submission of assignment

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