PHYS 3014: Statistical Mechanics

Lecture Notes
Part 3

Two Energy Levels System: Negative Temperature, Specific Heat

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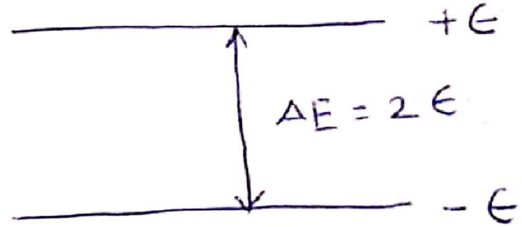
Two Energy Levels System : Negative Temperature, Specific heat

Consider a system consisting of N independent particles.



μ is the magnetic moment of each particle. They are either parallel or antiparallel to external field H. Let $+\epsilon$ and $-\epsilon$ are the energies associated with these orientations.

$$|\epsilon| = \mu H$$

Total energy of isolated system E can

be given as

$$E = n\epsilon = -N_{-}\epsilon + N_{+}\epsilon$$

where $n = N_{+} - N_{-}$, $N = N_{+} + N_{-}$

N_{+} have energies ϵ

N_{-} have energies $-\epsilon$

$\therefore$

$$N_{+} = \frac{1}{2}(N+n)$$

$$N_{-} = \frac{1}{2}(N-n)$$

The total no. of ways or arrangements $\Omega(n)$ corresponding to a net magnetic moment $M = n\mu$ and energy $E = n\epsilon$ is

$$\Omega(n) = \frac{\lfloor N}{\lfloor N_{-} \lfloor N_{+}}$$

So the no. of possible microstates corresponding to macroscopic conditions is $\Omega(n)$.

Equal volumes of phase space are associated with each independent arrangement of the magnetic moments. If this volume is unity then probability of occurence of a particular macrostate is $W(n) = \Omega(n)$.

Now

$$\ln W = \ln \lfloor N - \ln \lfloor N_+ - \ln \lfloor N_-$$

$$= N \ln N - N_+ \ln N_+ - N_- \ln N_-$$

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

We know that $\ln\left(1 \pm \frac{n}{N}\right) = \pm \frac{n}{N} - \frac{n^2}{2N^2} \pm \cdots$

$$\therefore \ln W = -\left[\frac{1}{2}N\left(1-\frac{n}{N}\right)\ln\frac{1}{2}\left(1-\frac{n}{N}\right) + \frac{1}{2}N\left(1+\frac{n}{N}\right) \ln\frac{1}{2}\left(1+\frac{n}{N}\right)\right]$$

$$\simeq -N_{-}\left[\ln\frac{1}{2} + \left(-\frac{n}{N} - \frac{n^2}{2N^2}\right)\right]$$

$$- N_{+}\left[\ln\frac{1}{2} + \left(\frac{n}{N} - \frac{n^2}{2N^2}\right)\right]$$

$$= -N\ln\frac{1}{2} - \frac{n^2}{2N}$$

Probability $\omega(M)$ of a Net Moment M

In zero magnetic field, each moment is equally likely to be $\pm u$.

For any specific arrangement, the

particle has probability $\frac{1}{2}$ for that orientation.

$\therefore$ probability that a specific arrangement of moments to occur is $\left(\frac{1}{2}\right)^N$.

So the probability $w(M)$ of a net moment M is

$$w(M) = \left(\frac{1}{2}\right)^N \cdot W(n)$$

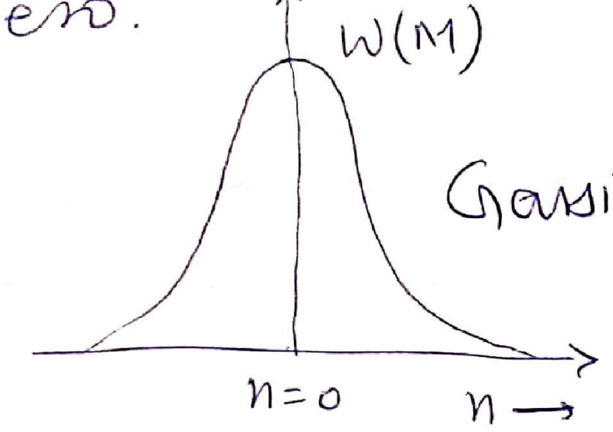
$$= \left(\frac{1}{2}\right)^N \exp\{\ln W(n)\}$$

$$= \left(\frac{1}{2}\right)^N \left[\left(\frac{1}{2}\right)^{-N} \exp\left(-\frac{n^2}{2N}\right)\right]$$

$$= \exp\left(-\frac{n^2}{2N}\right)$$

Magnetization has Gaussian distribution about the value $n=0$.

In the absence of external magnetic field, the average value of magnetization is zero.



Entropy

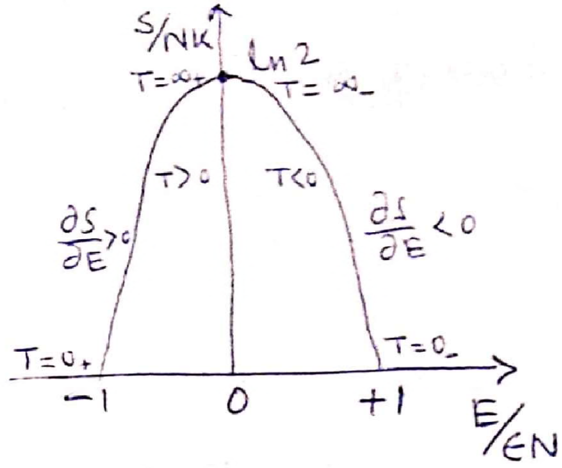
$$S = k \ln W$$

$$= -k\left[N_- \ln\left(\frac{N_-}{N}\right) + N_+ \ln\left(\frac{N_+}{N}\right)\right]$$

$$= -k\left[N \ln\frac{1}{2} + \frac{n^2}{2N}\right]$$

$$= -Nk\left[-\ln 2 + \frac{(E/\epsilon)^2}{2N^2}\right]$$

Plot of $\frac{S}{NK}$ with respect to $\frac{E}{\epsilon N}$ is shown in figure.



The slope $\frac{\partial S}{\partial E}$ gives the sign of temperature T.

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

$$= \frac{1}{\epsilon}\left(\frac{\partial S}{\partial n}\right)_{V,N} = \frac{1}{2}\frac{K}{\epsilon}\ln\left(\frac{N-n}{N+n}\right)$$

$$= \frac{1}{2}\frac{K}{\epsilon}\ln\left(\frac{N_-}{N_+}\right)$$

Negative Temperature

At conventional zero temperature, all particles are in ground state i.e in $-\epsilon$ and

$$n = N_+ - N_- = 0 - N = -N < 0$$

it gives $T = 0_+$ and $S = 0$

Complete order at $E = -N\epsilon$

As temperature increases or energy is given to the system, N_+ grows giving $T > 0$ till $n = 0$ where $S = Nk \ln 2$ maximum disorder and $T = \infty_+$.

If more energy is given to the system, population in upper level increases, i.e $N_+ > N_-$, $n > 0$

we get decrease in S more order and $T < 0$.

So the system is no longer in normal behaviour. This temperature i.e negative temperature T_- corresponds to higher energy than positive temperature T_+.

Further increasing energy given to the system, $n = N_+ - N_- = N - 0 = N > 0$

all particles in the upper state and $S = 0$ complete order and $T \doteq 0_-$

In the graph, at one side negative temperatures varies from $-\infty$ to -0 and positive temperatures varies from $+0$ to $+\infty$ is represented where $+\infty$ and $-\infty$ coincide with eachother.

specific heat

$$\frac{N+n}{N-n} = \frac{N_+}{N_-} \quad , \quad \Delta E = 2\epsilon$$

$$\frac{N_+}{N_-} = \exp\left(\frac{-2\epsilon}{kT}\right) = \exp\left(\frac{-\Delta E}{kT}\right)$$

$$\frac{N_-}{N} = \frac{\exp(\epsilon/kT)}{\exp\left(\frac{\epsilon}{kT}\right) + \exp\left(\frac{-\epsilon}{kT}\right)} = \frac{1}{1+\exp\left(\frac{-\Delta E}{kT}\right)}$$

$$\frac{N_+}{N} = \frac{\exp(+\epsilon/kT)}{\exp\left(\frac{\epsilon}{kT}\right) + \exp\left(\frac{-\epsilon}{kT}\right)} = \frac{1}{1+\exp\left(\frac{\Delta E}{kT}\right)}$$

energy $E = n\epsilon = -(N_- - N_+)\epsilon$

$$= -N\epsilon \tanh\left(\frac{\epsilon}{kT}\right)$$

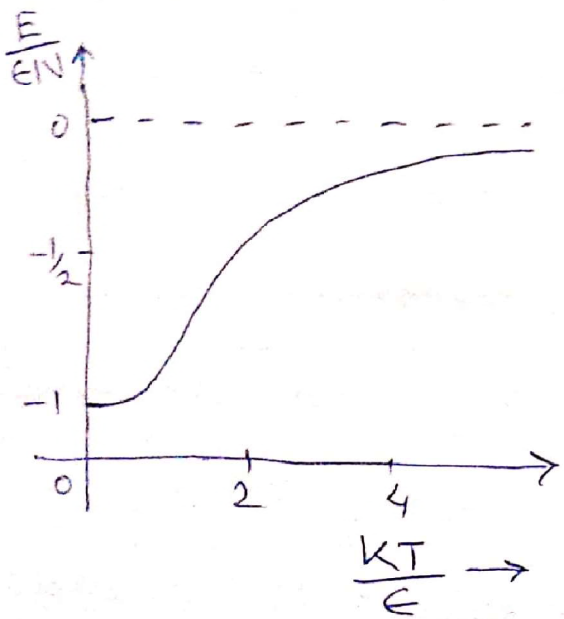
Specific heat

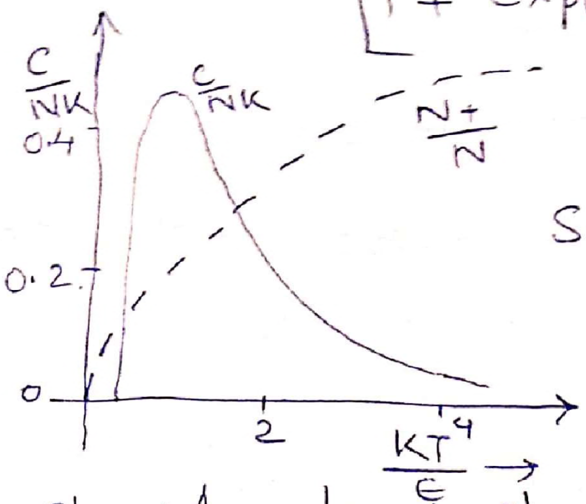
$$C = \frac{dE}{dT}$$

$$= NK \frac{\left(\frac{\epsilon}{KT}\right)^2}{\cosh^2\left(\frac{\epsilon}{KT}\right)}$$

$$= NK \frac{4\left(\frac{\epsilon}{KT}\right)^2}{\left[\exp\left(\frac{\epsilon}{KT}\right) + \exp\left(\frac{-\epsilon}{KT}\right)\right]^2}$$

$$= NK\left(\frac{\Delta E}{KT}\right)^2 \frac{\exp\left(\frac{\Delta E}{KT}\right)}{\left[1 + \exp\left(\frac{\Delta E}{KT}\right)\right]^2}$$





Schottky anomaly
specific heat
show a peak.

Specific heat shows a peak
when body has a gap ΔE in
its energy states.

References:

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- Statistical Mechanics by B. K. Agarwal and M. Eisner
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- Elementary Statistical Physics by C. Kittel
- Fundamentals of Statistical and Thermal Physics by F. Reif
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Thank You

For any questions/doubts/suggestions and submission of assignments

Write at E-mail: akgupta@mgcub.ac.in