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THE STUDY OF PARTITION FUNCTION, OCCUPATION NUMBER, INTERNAL ENERGY AND ENTROPY USING SCILAB

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ABSTRACT: -

The study of partition function, occupation number, internal energy and entropy using scilab has been done. All the plots are labelled and variation with temperature is shown in the figures. The results for the occupation number (n) partition function, occupation number, internal energy and entropy are well defined and interpreted, for the first excited state n increases and decreases for the ground state. Due to dipoles orientation at high T total internal energy goes to zero. The entropy becomes maximum and the system tends to equilibrium when T is increased.

KEYWORDS: Scilab and statistical parameters

INTRODUCTION:

Scilab is an open source platform there is no requirement to purchase it because it is free software. The graphics play very important role inbuilt-in Scilab/Matlab. This is the strongest features (property) of this software. But in other Softwares or languages like C, C+, C++ and Fortran are generally text-based. Scilab provides a complete environment in where the graphical routines are an integral component and consistent across different operating systems. The Installation of this software is so easy and it does not require more space as like other Softwares. The operations of the Scilab are similar to Matlab. Algorithm is very important in Scilab in other words we can that it is procedure of developed codes. The problem based on Euler's method and modify Euler's method were solved using Scilab [1]. The comparison of Harmonic Euler's and the modified Euler's method was done by Qureshi et.al. [2]. It is very easy to solve the differential equations either linear or non-linear by Scilab. The approximation solution of the differential equations using initial value problems was compared of the with the exact solution [3]. The study of M-B distribution, F-D distribution and B-E distribution with the energy at different temperatures was done [4]. Using essential computing tools the discussion of brief history of Fermi-Dirac statistics took place [5]. The electron trajectory problem was solved Scilab Xcos [6]. The problem based on weighted least square method was done using Scilab [7]. For the data representation for the geophysical observations and output of the numerical model was studied for a best fit straight line in the geosciences [8]. Two algorithms with active-set strategies and novel precision-parameter for the adjustment schemes were represented and the outcomes of algorithms are found competitive with other algorithms from the literature [9]. The kernel of the application developed by open technologies using SciLab/Xcos environment [10]. Using open source software the rapid controller prototyping environment had been presented [11]. Author reviews that Scilab can be used for data analysis as well as applied numerical work which can be useful in research and teaching [12]. The study on NARVAL module had been done and using Scilab simulate the AODV [13]. The partition function *Z* plays very important role in statistical mechanics which encodes the statistical properties of a system in thermodynamic equilibrium and other parameters such as entropy, energy and specific heat etc. can be constructed by Z. The relation between the thermodynamics and the quantum theory of black hole horizons through the thermodynamic partition function which was based on some physically plausible arguments partly [14].

In this paper we take into account a system of N non-interacting particles in equilibrium. Suppose we have two energy levels, say one is E_1 with N_1 particles and other E_2 which has N_2 particles. Particles N_1 are oriented parallel to the magnetic field (B) and N_2 are anti-parallel to magnetic field (B). In this paper we plot Partition Function (Z), Occupation number (n), Internal energy and Specific Heat with Temperature (T). Here we are discussing only for two levels as already explained. The formulae for above parameters are given below with the symbol meanings.

The partition function is given by the formula $Z = [2*\cosh\{(\mu*B)/(k_b*T)\}]$

The occupation number is given by the formula

$$n = (\exp((\mu*B)/(k_b*T)))/(2*\cosh((\mu*B)/(k_b*T)))$$

The internal energy is given by the formula $E= - \mu*B*\tanh\{(\mu*B)/(k_b*T))\}$

The entropy energy is given by the formula

$$S = k_b*[\log(2*\cosh\{(\mu*B)/(k_b*T)\}] - [(\mu*B)/(k_b*T))*\tanh\{(\mu*B)/(k_b*T)\}]$$

Where k_b is the Boltzmann's Constant.

B is the Magnetic field; T is the Absolute temperature; μ is the Chemical Potential and S is the entropy.

Algorithm:

1. First we put the values of all constants such as of μ, B, k_B etc.
2. Now define two array and for two different temperature ranges such that T=linspace(0.1,10,1500) and T1=linspace(1,10,1500).
3. Using **for loop** we make array of points for smooth curve..
4. Use plot commands with style, marker and line.
5. Labelling the graphs using commands.

SCILAB CODES:

```
clf
clear
B=0.5 //Tesla
K=8.617e-5 // It is Boltzamann constant in eV/K
mu=5.78e-5 //eV/Tesla
T=linspace(0.1,10,1500)
T1=linspace(1,10,1500)
for i=1:1500
Z(i)=2*cosh((mu*B)/(K*T(i))) // represents the partition function
Z1(i)=2*cosh((mu*B)/(K*T1(i))) // represents the partition function
N1(i)=(exp((mu*B)/(K*T(i))))/(2*cosh((mu*B)/(K*T(i)))) // represents the occupation
number for ground state in the program
N2(i)=(exp(-(mu*B)/(K*T(i))))/(2*cosh((mu*B)/(K*T(i)))) //Occupation Number for Excited
State
SH(i)=(K*(((mu*B)./(K*T(i))).^2)*(sech((mu*B)./(K*T(i)))).^2) //represents the specific
heat
E(i)=-mu*B*tanh((mu*B)/(K*T(i))) // represents the internal energy
E1(i)=K*(log(2*cosh((mu*B)/(K*T(i))))-((mu*B)/(K*T(i)))*tanh((mu*B)/(K*T(i)))) //
represents the entropy
end

scf(0)
plot(T',Z,'r','linewidth',3)
ylabel('$\boldsymbol{N\rightarrow}\$','fontsize',5)
xlabel('$\boldsymbol{Temperature\rightarrow}\$','fontsize',5)
legend('Range of T = 0.1K to 1.5K')

scf(1)
plot(T1',Z1,'g','linewidth',3)
ylabel('$\boldsymbol{N\rightarrow}\$','fontsize',4)
xlabel('$\boldsymbol{Temperature\rightarrow}\$','fontsize',5)
title('Partition function (Z)','fontsize',5 )
legend('Range of T = 1K to 15K')
```

```
scf(2)
plot(T',N1,'b','linewidth',3)
plot(T',N2,'c','linewidth',3)
ylabel('$\boldsymbol{n\rightarrow}\$','fontsize',5)
xlabel('$\boldsymbol{Temperature\rightarrow}\$','fontsize',5)
title('Occupation Number(n) for Ground state and Excited state','fontsize',5 )
legend('For n1 = N1/N','For n2 = N2/N',4)

scf(3)
plot(T',E,'c','linewidth',3)
ylabel('$\boldsymbol{U/N\rightarrow}\$','fontsize',5)
xlabel('$\boldsymbol{Temperature\rightarrow}\$','fontsize',5)
title('Internal Energy (E)','fontsize',5 )
legend('Range of T = 1K to 15K',4)

scf(4)
plot(T',E1,'m','linewidth',3)
ylabel('$\boldsymbol{S/N\rightarrow}\$','fontsize',5)
xlabel('$\boldsymbol{Temperature\rightarrow}\$','fontsize',5)
title('Entropy (S)','fontsize',5 )
legend('Range of T = 1K to 15K',4)
```

OUTPUTS:

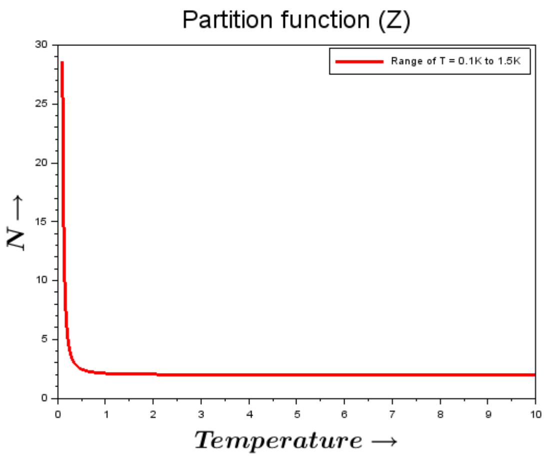

Figure (1)

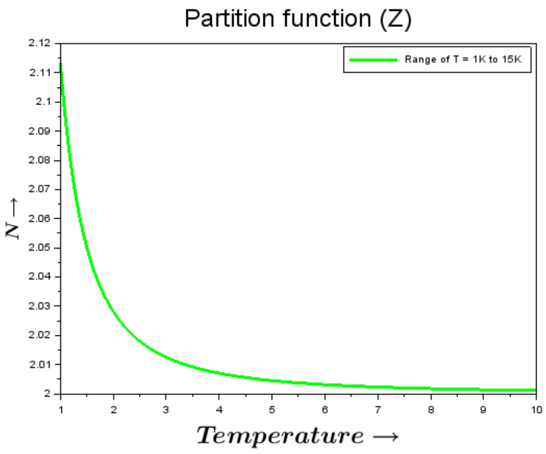

Figure (2)

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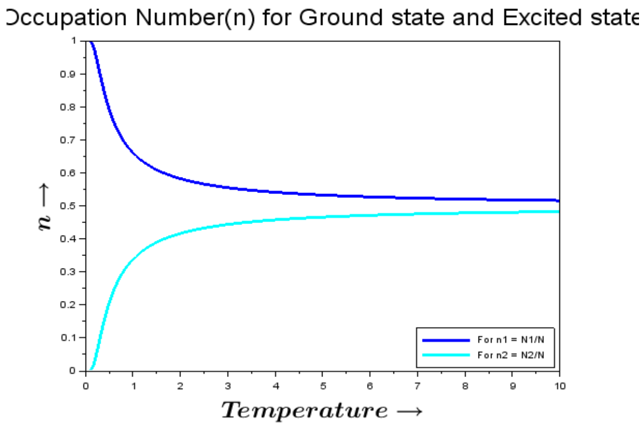

Figure (3)

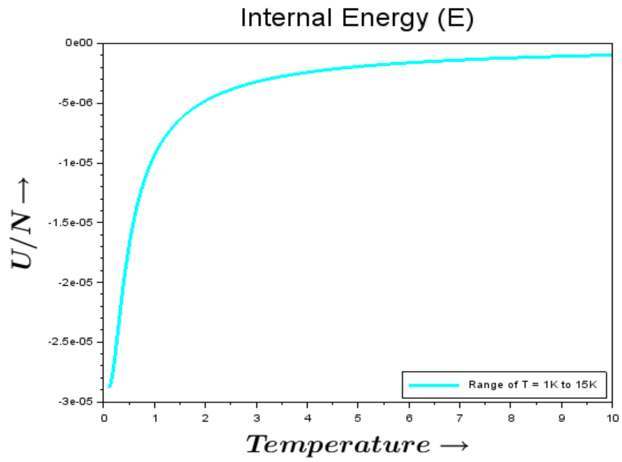

Figure (4)

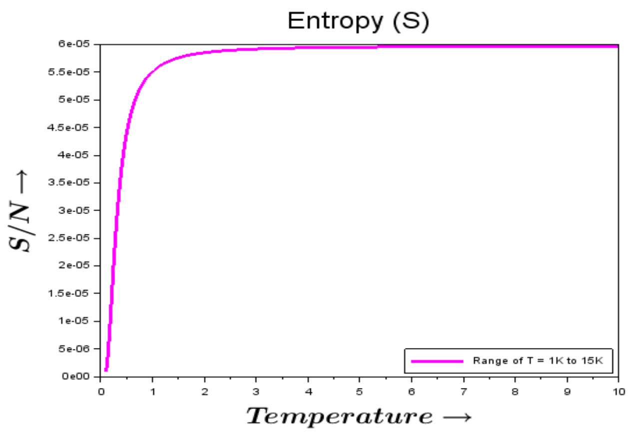

Figure (5)

RESULTS AND CONCLUSIONS:

The Scicodes have been done successfully. All the plots are labelled and variation with temperature is shown in the figures. For the occupation number (n) it is found that at 0K, all the particles are in ground state so n tends to 1 again on increasing the temperature, the energy gained by the particle then excited; for the first excited state n increases and decreases for the ground state. For 0 K in the field direction dipoles are oriented results in is negative energy (-µ.B) and opposite for antiparallel so at high T total internal energy goes to zero. The entropy becomes maximum and the system tends to equilibrium when T is increased. In this paper all the plots has been studied by Scilab. Scilab having much more application in science branch viz. Physics, Computational field and all the branches of sciences. It's free software.

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