

TN2624 MATLAB Session 4

March 7, 2013

Heat capacity of the Einstein solid – numerical calculations (50 pts)

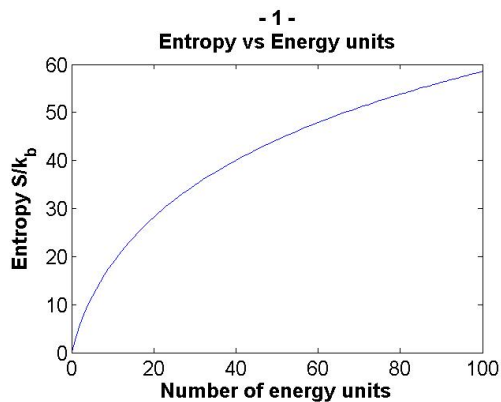
1. (10 pts)

$$\Omega(N, q) = \frac{(q + N - 1)!}{q!(N - 1)!}$$

(2points)

```
clear all
clc
N=25;
q=0:100;
sok=gamma1n(q+N)-gamma1n(q+1)-ones(1,length(q)).*gamma1n(N)
```

(4points)



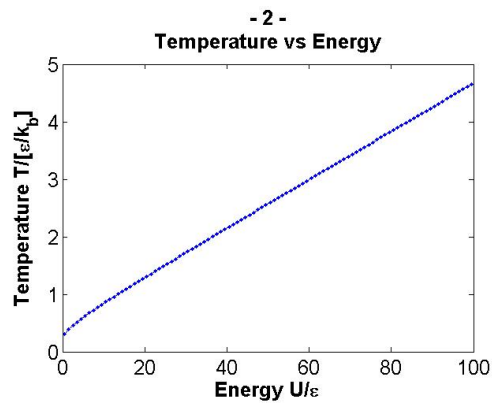
(4points), no labels: (2points)

2. (10 pts)

The resulting temperature has units ϵ/k_b (2points)

```
U=q; %Energy in units of epsilon
T=diff(U)./diff(sok)
%Interpolate the vector U
Uint=(diff(U)*0.5+U(1:(end-1)))
```

(4points)

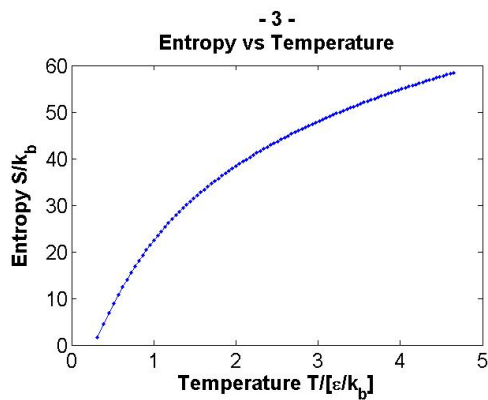


(4points), no labels: (-2points)

3. (10 pts)

```
%Interpolate the vector sok
sokint=(diff(sok)*0.5+sok(1:(end-1)))
```

(0points)



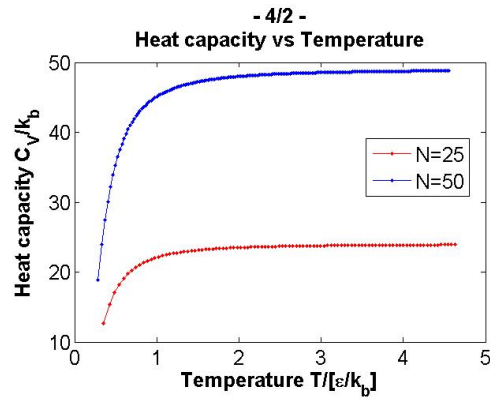
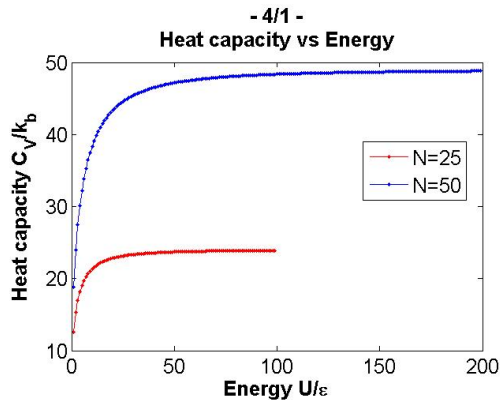
(10points), no labels: (-2 points)

4. (20 pts)

The units of the heat capacity is just k_b . (2 points)

```
C=diff(Uint)./diff(T)
Tint=(diff(T)*0.5+T(1:(end-1)))
Uint2=(diff(Uint)*0.5+Uint(1:(end-1)))
```

(6 points)



(6points per plot); no labels (-2 points per plot); no legend (-2 points per plot)

A larger number of oscillators leads to a higher heat capacity. (3points) Larger number of oscillators \rightarrow higher multiplicity and entropy \rightarrow larger slope of the function $S(U) \rightarrow$ lower maximum temperature for a given energy range OR higher heat capacity \rightarrow lower temperature for given internal energy OR any other explanation (3points)

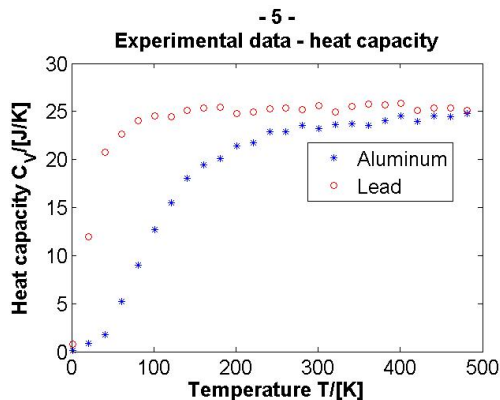
Heat capacity of the Einstein solid – comparison to real examples (50 pts)

5. (15 pts)

```
clear all
clc
```

```
A_Pb=importdata('lead.dat');
C_Pb=A_Pb(:,2);
T_Pb=A_Pb(:,1);
```

```
A_Al=importdata('aluminum.dat');
C_Al=A_Al(:,2);
T_Al=A_Al(:,1);
```



(15points), no legend: (-4points), no labels: (-4points)

6. (20 pts)

```

T_exp=T_Pb;
C_exp=C_Pb;
%T_exp=T_Al;
%C_exp=C_Al;

Na=6.022*10^23;
kb=1.38*10^-23; %J/K
ev=1.6*10^-19;
C_func=@(eps) sum((C_exp-3*Na*kb.*(eps./(kb.*T_exp)).^2.*...
    exp(eps./(kb.*T_exp))./(exp(eps./(kb.*T_exp))-1).^2).^2)

epsf=fminsearch(C_func,0.01*ev)/ev

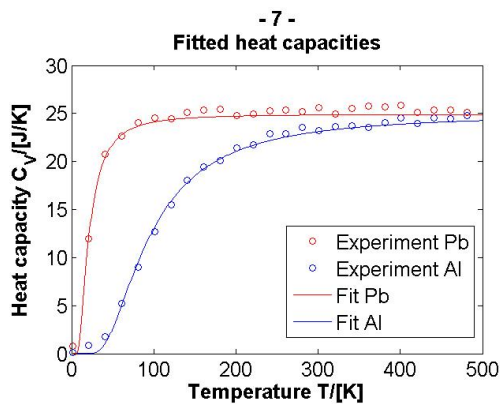
```

(14points)

$\epsilon_{Pb} = 0.0055 \text{ eV}$ **(3points)**

$\epsilon_{Al} = 0.0248 \text{ eV}$ **(3points)**

7. **(10 pts)**



(10points), no legend: **(-2points)**, no labels: **(-2points)**

8. **(5 pts)**

The distance between the energy levels is proportional to the frequency f of the oscillator $\epsilon = hf$. h is Planck's constant. Therefore, higher values of ϵ are an indication for higher frequencies, higher spring constants, and therefore for stiffer/harder materials/higher speed of sound. **(5points)**