Lecture

Microcanonical distribution

The states $j = (j_1, \dots, j_N)$ for the paramagnet can be grouped in classes that have the same energy E_j

$$E_j = -(j_1 + \dots + j_N)\, B$$

For example for $N = 4$

	$\Uparrow B$		Number of states
State 1	↓↓↓↓	$E_1 = 4B$	$1 = \binom{4}{0}$
State 2	↑↓↓↓	$E_2 = 3B - B = 2B$	
State 3	↓↑↓↓	$E_3 = 3B - B = 2B$	$4 = \binom{4}{1}$
State 4	↓↓↑↓	$E_4 = 3B - B = 2B$	
State 5	↓↓↓↑	$E_5 = 3B - B = 2B$	
State 6	↑↑↓↓	$E_6 = 2B - 2B = 0$	
State 7	↑↓↑↓	$E_7 = 2B - 2B = 0$	
State 8	↑↓↓↑	$E_8 = 2B - 2B = 0$	$6 = \binom{4}{2}$
State 9	↓↑↑↓	$E_9 = 2B - 2B = 0$	
State 10	↓↑↓↑	$E_{10} = 2B - 2B = 0$	
State 11	↓↓↑↑	$E_{11} = 2B - 2B = 0$	

	Configuration	Energy	Number of states
State 12	↑↑↑↓	$E_{12} = -3B + B = -2B$	
State 13	↑↓↑↑	$E_{13} = -3B + B = -2B$	$4 = \binom{4}{3}$
State 14	↑↑↓↑	$E_{14} = -3B + B = -2B$	
State 15	↓↑↑↑	$E_{15} = -3B + B = -2B$	
State 16	↑↑↑↑	$E_{16} = -4B$	$1 = \binom{4}{4}$

A representation of the <u>energy levels</u> (which is <u>less complete</u> in comparison with a complete list of all configurations) is

		Number of states
$E_{group 1} = 4B$	————	$\binom{4}{0}$
$E_{group 2} = 2B$	————	$\binom{4}{1}$
$E_{group 3} = 0$	————	$\binom{4}{2}$
$E_{group 4} = -2B$	————	$\binom{4}{3}$
$E_{group 5} = -4B$	————	$\binom{4}{4}$

The partition function is

$$Z = 1 \cdot e^{-\beta 4B} + 4 \cdot e^{-\beta \cdot 2B} + 6 \cdot e^{-\beta \cdot 0} + 4 e^{\beta 2B} + + e^{\beta 4B}$$

In general, for N magnetic dipoles

$$Z = \binom{N}{0} e^{-\beta \cdot NB} + \binom{N}{1} e^{-\beta(N-2)B} + \binom{N}{2} e^{-\beta(N-4)B} +$$

$$\cdots + \binom{N}{n} e^{-\beta(N-2n)B} + \cdots + \binom{N}{N} e^{-\beta(N-2N)B}$$

The binomial coefficients $\binom{N}{n}$ represent the number of states corresponding to the energy level $E = (N-2n)B$. It is also called the degeneracy of the energy level. In statistical physics it is dinoted by

$\Omega(E)$

or $W(E)$

or $g(E)$

So

$$Z = \sum_{\text{ENERGY LEVELS}} \Omega(E)\, e^{-\beta E}$$

Notice that here the sum is over ENERGY LEVELS and not over ALL STATES.

Not paying attention to this difference in the summation index can cause big confusions.

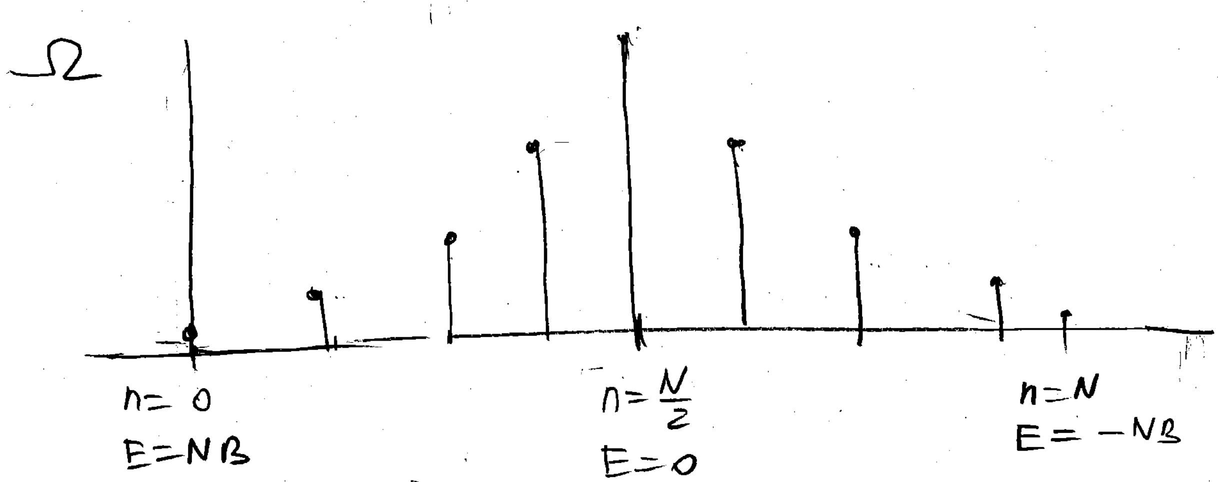
For our paramagnet case

$$\Omega(E) = \binom{N}{n}$$

with $E = (N-2n)B$

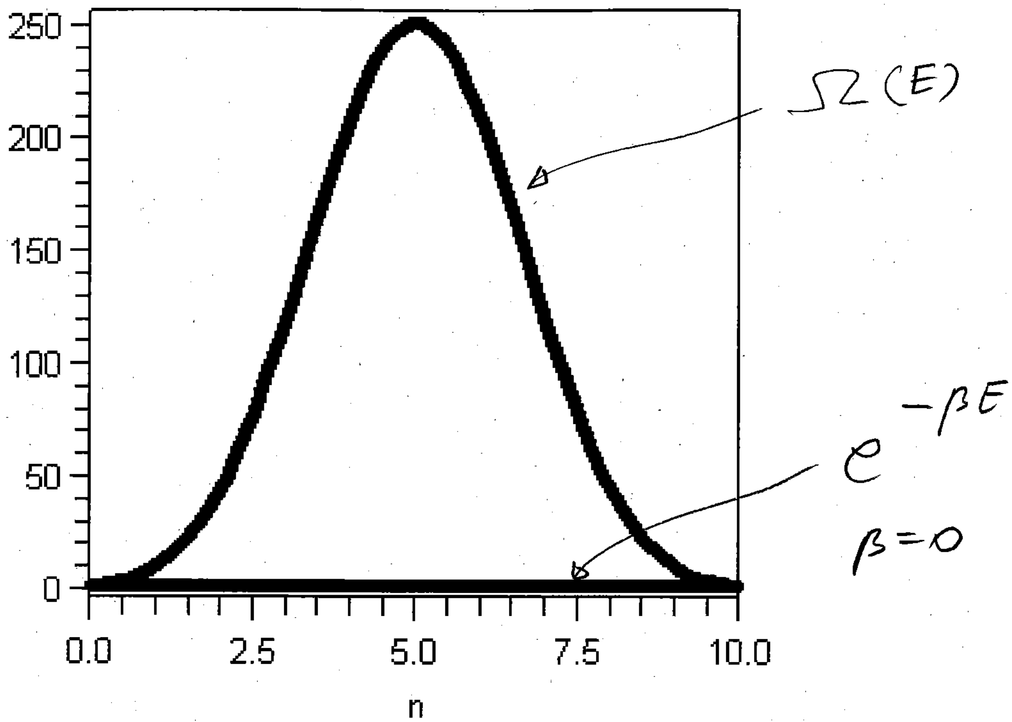
The integer n enumerates the energy levels and takes the values $0, 1, 2, \ldots N$

We notice that $\Omega(E)$ are the binomial coefficients. Thus $\Omega(E)$ will take the maximum value at $n = \frac{N}{2}$



$$\Omega(E) = \binom{N}{n} \qquad E = (N-2n)B$$

```
> with(plots):display([plot(subs(N=10,exp(-0.00*(N-2*n))),n=0..10,
  color=blue),plot(subs(N=10,N!/(n!*(N-n)!)), n=0..10)]);
```




```
> plot(subs(N=10,N!/(n!*(N-n)!)*exp(-0.00*(N-2*n))), n=0..10);
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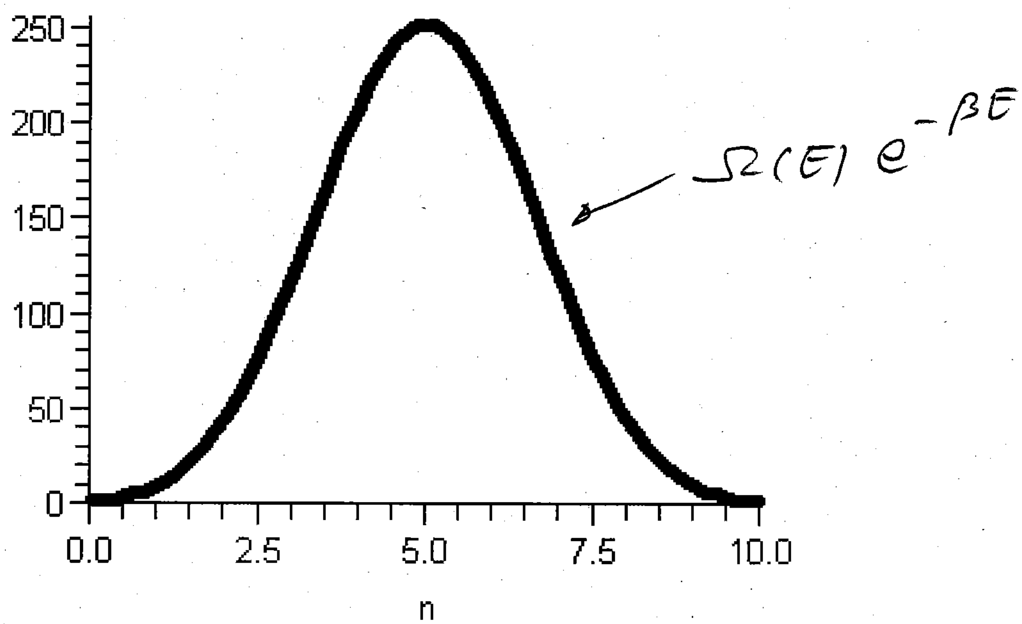
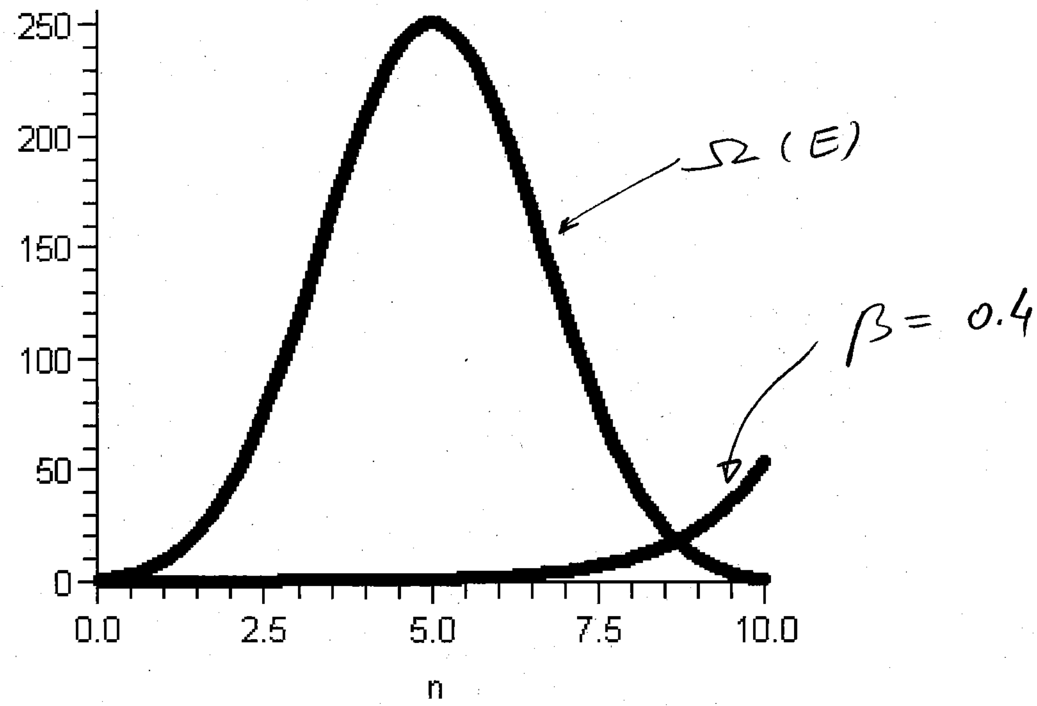


```
> with(plots):display([plot(subs(N=10,exp(-0.4*(N-2*n))),n=0..10,
  color=blue),plot(subs(N=10,N!/(n!*(N-n)!)), n=0..10)]);
```




```
> plot(subs(N=10,N!/(n!*(N-n)!)*exp(-0.4*(N-2*n))), n=0..10);
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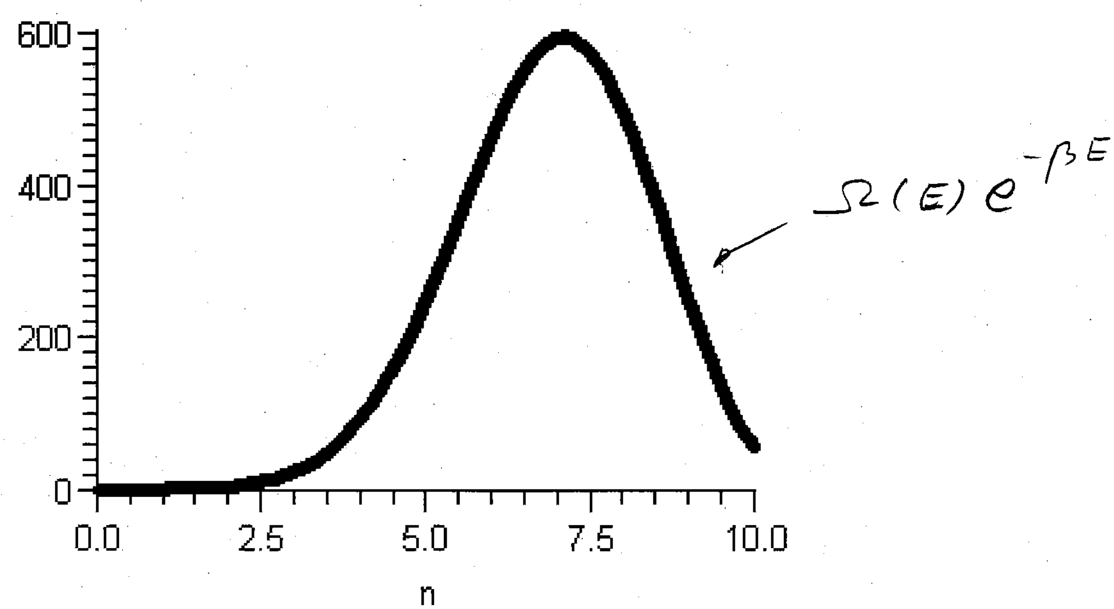
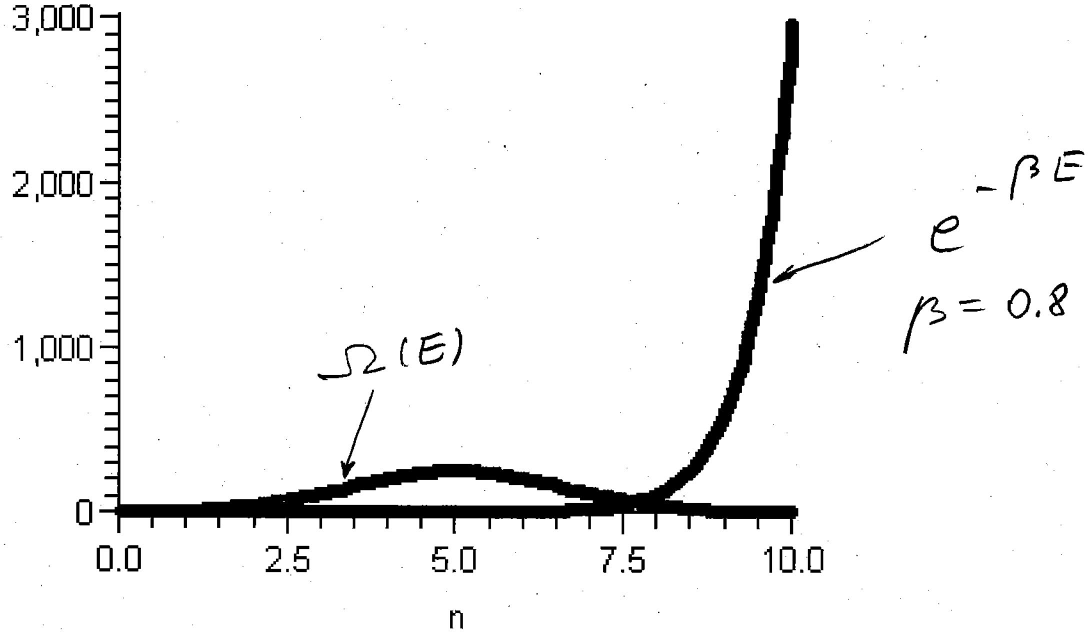


```
> with(plots):display([plot(subs(N=10,exp(-0.8*(N-2*n))),n=0..10,
  color=blue),plot(subs(N=10,N!/(n!*(N-n)!)), n=0..10)]);
```




```
> plot(subs(N=10,N!/(n!*(N-n)!)*exp(-0.8*(N-2*n))), n=0..10);
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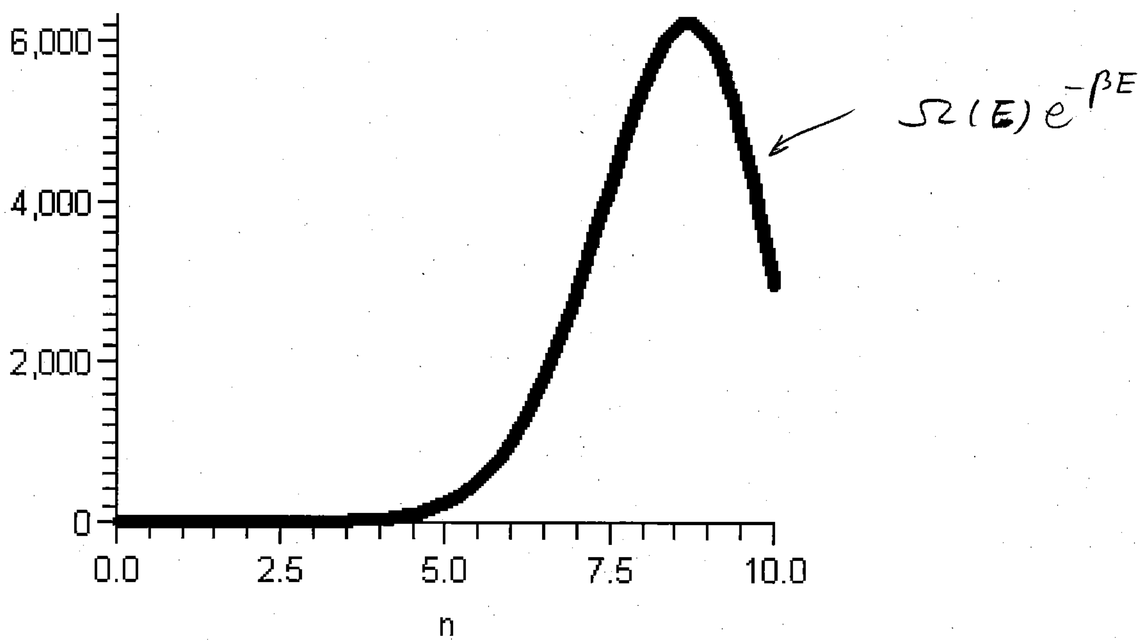

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> with(plots):display([plot(subs(N=10,exp(-1.2*(N-2*n))),n=0..10,
  color=blue),plot(subs(N=10,N!/(n!*(N-n)!)), n=0..10)]);
```

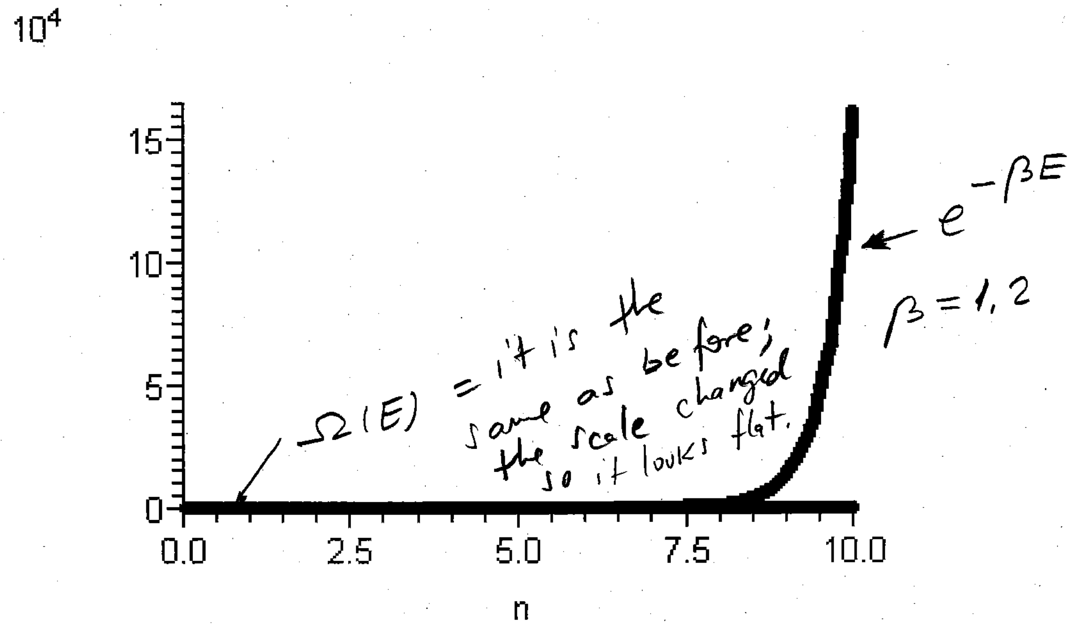


```
> plot(subs(N=10,N!/(n!*(N-n)!)*exp(-1.2*(N-2*n))), n=0..10);
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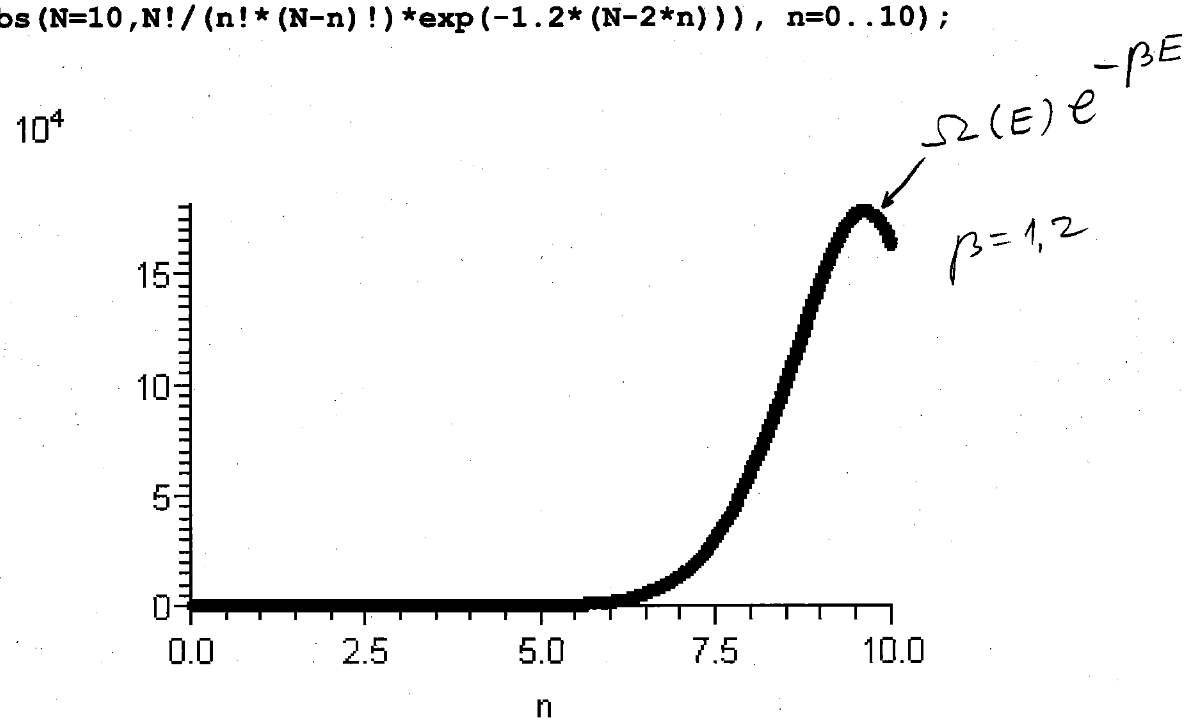

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> with(plots):display([plot(subs(N=10,exp(-2*(N-2*n))),n=0..10,
  color=blue),plot(subs(N=10,N!/(n!*(N-n)!)), n=0..10)]);
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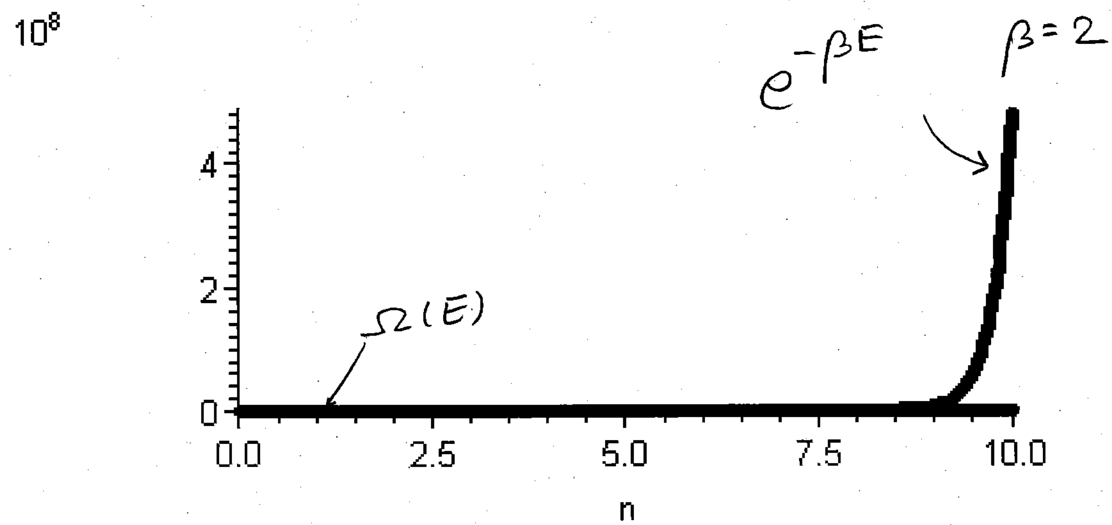


```
> plot(subs(N=10,N!/(n!*(N-n)!)*exp(-2*(N-2*n))), n=0..10);
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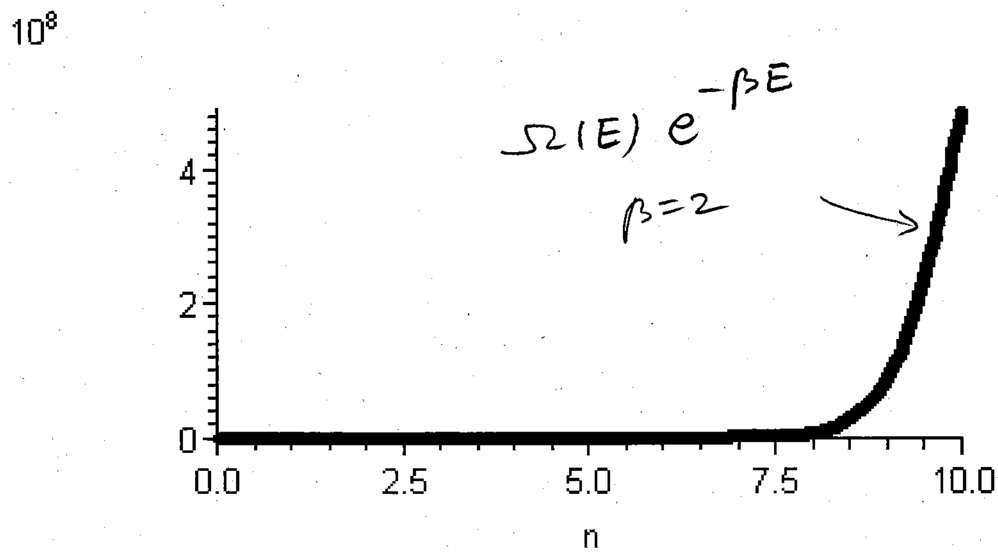


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>
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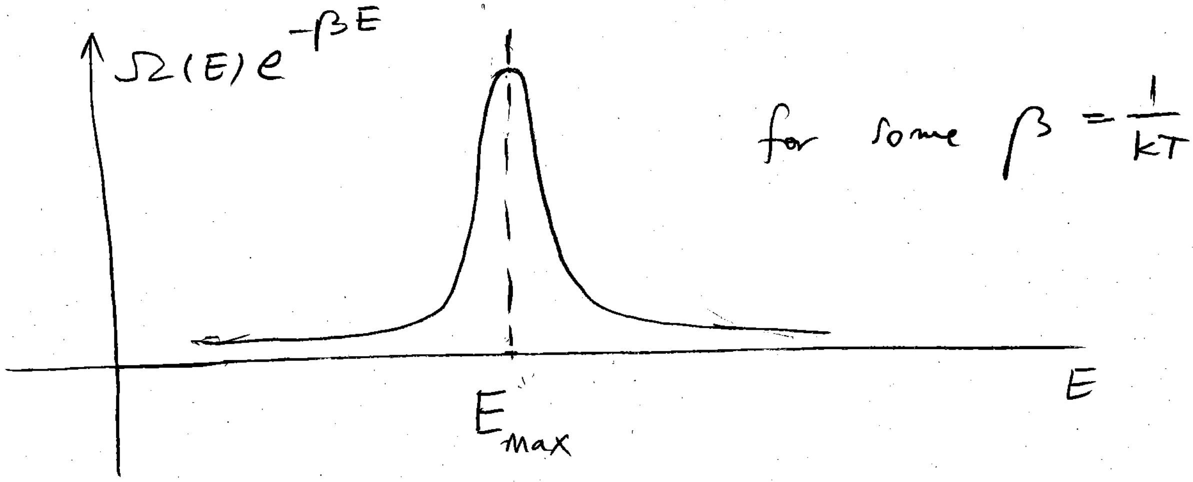
Consider the temperature T in a range such that $\Omega(E)\, e^{-\beta E}$ is belled shaped



For such temperatures we can approximate

$$Z = \sum_{\substack{\text{energy} \\ \text{levels}}} \Omega(E)\, e^{-\beta E} \simeq \Omega(E_{max})\, e^{-\beta E_{max}}$$

where E_{max} is the solution to the equation

$$\frac{d}{dE}\left(\Omega(E)\, e^{-\beta E}\right) = 0 \qquad (1)$$

The procedure for finding Z for this temperature range is thus as follows:

Step 1

Find E_{max} from $\frac{d}{dE}\left(\Omega(E)\, e^{-\beta E}\right) = 0$

Step 2

$$Z = \Omega(E_{max})\, e^{-\beta E_{max}}$$

We can elaborate Step 1 and give it a physical meaning.

$$\frac{d}{dE}\left(\Omega(E)\, e^{-\beta E}\right) = \frac{d}{dE}\left(\Omega(E)\right) e^{-\beta E} - \beta\, \Omega(E)\, e^{-\beta E}$$

the condition for E_{max} is thus

$$\frac{d}{dE}\left(\Omega(E)\right) = \beta\, \Omega(E)$$

or

$$\frac{1}{\Omega(E)} \frac{d\left(\Omega(E)\right)}{dE} = \beta$$

$$\frac{d \ln \Omega(E)}{dE} = \beta$$

(*) $$\boxed{\frac{d}{dE}\left[k \ln \Omega(E)\right] = \frac{1}{T}}$$ Condition to find E_{max} given T

In our present approximation only the energy level E_{max} is important, all the other were neglected. Is as if we isolated the system from the heat bath and thus it has a constant energy E_{max}

$$\boxed{\text{Isolated system at } E_{max}}$$

The states of the system are now constrained by the condition

$$E = \text{constant} = E_{max}$$

The state index j takes $\Omega(E_{max})$ values

$$j = 1, 2, \dots, \Omega(E_{max}).$$

Each state has the SAME PROBABILITY to appear (they all have the same energy!)

$$P_j = \frac{e^{-\beta E_{max}}}{Z} = \frac{e^{-\beta E_{max}}}{\Omega(E_{max})\, e^{-\beta E_{max}}}$$

MICROCANONICAL DISTRIBUTION

$$\boxed{P_j = \frac{1}{\Omega(E_{max})}, \quad j = 1, 2, \dots \Omega(E_{max})}$$

The entropy in this case reduces to

$$S = -k \sum_{j=1}^{\Omega(E_{max})} P_j \ln P_j =$$

$$= -k\, \Omega(E_{max})\, P_j \ln P_j =$$

all P_j are equal

$$= -k\, \cancel{\Omega(E_{max})} \frac{1}{\cancel{\Omega(E_{max})}} \ln \frac{1}{\Omega(E_{max})} =$$

$$= -k \ln \frac{1}{\Omega(E_{max})} =$$

$$= k \ln \Omega(E_{max})$$

notice that here the sign is positive

$$\boxed{S = k \ln \Omega(E_{max})}$$ for microcanonical distribution

The condition (*) becomes thus

$$\boxed{\frac{1}{T} = \frac{dS}{dE}}$$

Condition to find E_{max} given T.

Conclusion: Microcanonical distribution

(1) Find the number of states for each energy E:

$$\Omega(E)$$

(2) Find the Boltzmann entropy (this is the name for the entropy for the microcanonical distribution; we call it Gibbs entropy for the canonical distribution)

$$S = k \ln \Omega(E)$$

(3) Find the thermodynamic relation

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E}\right)_{\text{at some constant thermodynamic state parameters}}$$

we will add other thermodynamic relation later.