Statistical Mechanics for Neural Networks and Deep Learning

with

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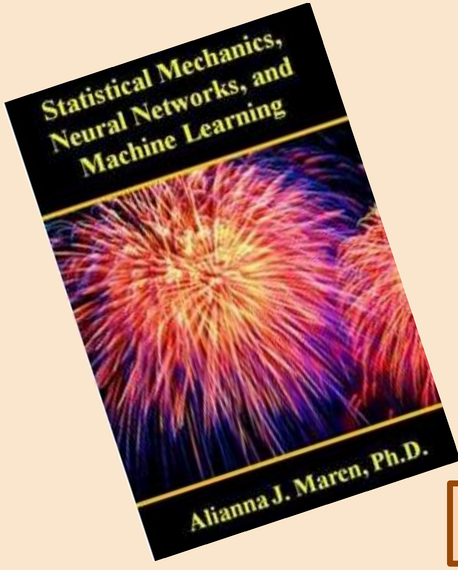
Microstates and Partition Functions: *Some Simple Examples*



Author's Note:

The following material accompanies the *Précis* for the book-in-progress, **Statistical Mechanics for Neural Networks and Deep Learning**.
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Microstates : A Series of Examples

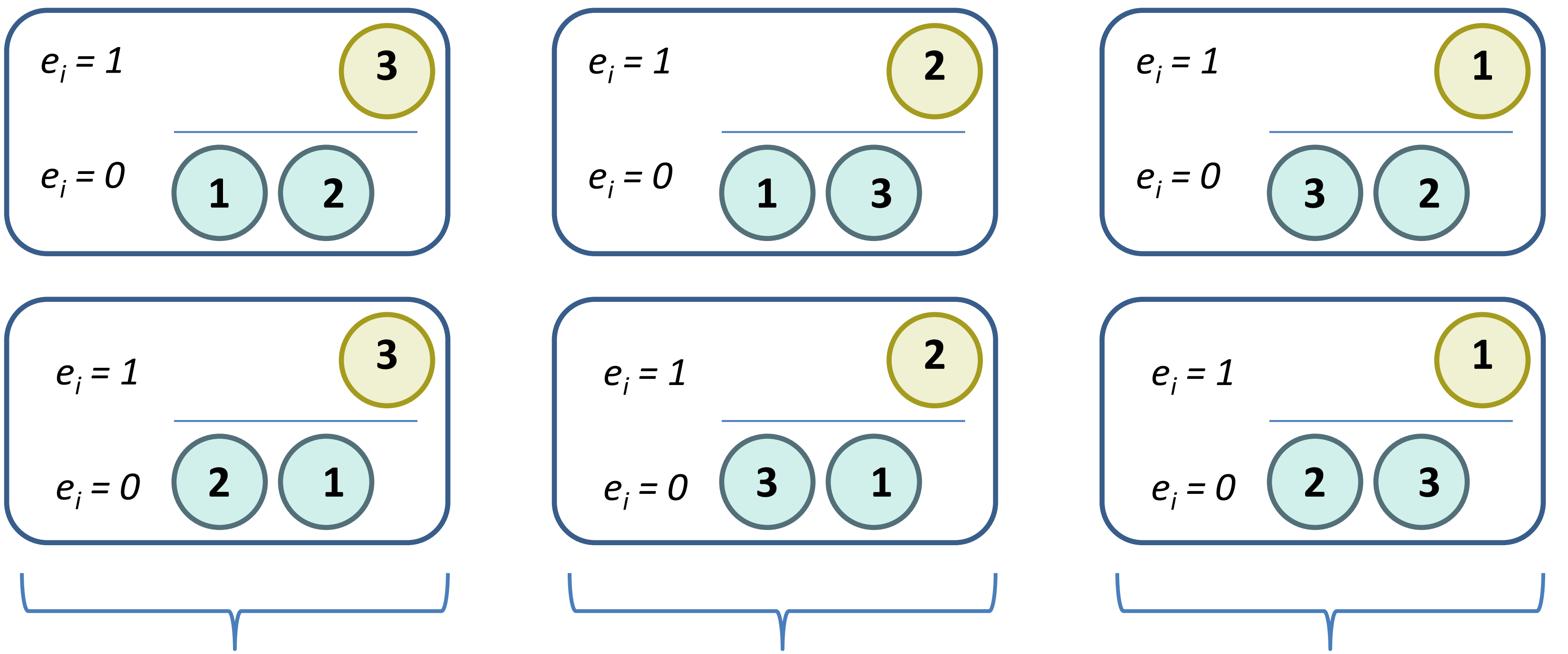
Example 1:

For a System with Three Units and Two Energy Levels;

A Single Microstate:

Two Units in Level $e_i = 0$, One Unit in Level $e_i = 1$

We can create six different nominal configurations:



These two microstates are identical These two microstates are identical These two microstates are identical

Microstates, Example 1 (2)

*We can create three different **non-identical** configurations*

- Total ways of distributing the N units among the N different total spots: $N!$
  - Total number of spots available (same as total number of units): N
  - Choice of N different units to fill the first spot: Here, $N = 3$.
  - Choice of $N-1$ different (remaining) units to fill the next spot: Here, $N-1 = 2$.
  - Choice of $N-2$ different (remaining) units to fill the next spot: Here, $N-2 = 1$.
  - Total number of ways of distributing the $N = 3$ units: 3*2*1 = 6.
  - These six configurations contain *some which are identical* with the others.

- Number of units going into Level $e_i = 1$ (or e_1): 1
  - $N_1 = 1$; there is just one spot at e_1; this means that there is no way to have a problem distinguishing among multiple units – there's only one unit there!
  - Just for formality's sake, we can create the term $N_1! = 1! = 1$.

- Number of ways of populating Level $e_i = 0$ (or e_0): 4
  - After we've put one of the units into Level e_1, there are $N_2 = N - N_1$ units left. (Here, $N_2 = 2$.)
  - The way in which we can multiply count the same configuration (the degeneracy) is $N_2! = 2! = 2$.

Number of *countably different* ways of populating the two states:

$$Z = \frac{N!}{N_1!\,N_2!} = \frac{3*2*1}{1!*2!} = \frac{6}{2} = 3$$

Microstates; Example 1 (3)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Total Accessible Microstates
1	3	0	1
2	2	1	3
3	1	2	3
4	0	3	1

Total number of distinct, accessible microstates: 8

Microstates; Example 1 (4)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Computing the probability distribution

Example 1(a): Suppose that the energy of $e_0 = 0$, and the energy of $e_1 = 1$

$$p_j = \exp(-\beta E_j)/Z$$

where j refers to a specific microstate, and E_j is the energy of that microstate. Let $\beta = 1$

Z, the normalization constant, is the partition function

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Energy for that Microstate	Total Energy for that Microstate	$exp(-E_j)$ for that Microstate	*N = Total Accessible Instances of that Microstate*	$exp(-E_j) * N$
1	3	0	3*0 + 0*1	0	1	1	1.000
2	2	1	2*0 + 1*1	1	0.368	3	1.104
3	1	2	1*0 + 2*1	2	0.135	3	0.405
4	0	3	0*0 + 3*1	3	0.050	1	0.050

Sum of all the p_j*Z*N: 1.000 + 1.104 + 0.405 + 0.050 = 2.559

Microstates; Example 1 (5)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Computing the probability distribution

$$1 = \frac{1}{Z}\sum_j p_j = \frac{1}{Z}\sum_j \exp(-\beta E_j)$$

$$Z = \sum_j \exp(-\beta E_j)$$

Sum of all the exp($-E_j$)*N: 1.000 + 1.104 + 0.405 + 0.050 = 2.559
Z = 2.559

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Total E_j Energy for that Microstate	*exp($-E_j$)* for that Microstate	*N = Total Accessible Microstate Instances*	p_j = *exp($-E_j$) * N/Z*
1	3	0	0	1	1	1.000/2.559 = 0.391
2	2	1	1	0.368	3	1.104/2.559 = 0.431
3	1	2	2	0.135	3	0.405/2.559 = 0.158
4	0	3	3	0.050	1	0.050/2.559 = 0.020

Sum of all p_j: 0.391 + 0.431 + 0.158 + 0.020 = 1.000
(Sum of the probabilities = 1)

Microstates; Example 1 (6)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Total Energy for that Microstate	$exp(-E_j)$ for that Microstate	*N = Total Accessible Microstate Instances*	$p_j = exp(-E_j) * N/Z$
1	3	0	0	1	1	0.391
2	2	1	1	0.368	3	0.431
3	1	2	2	0.135	3	0.158
4	0	3	3	0.050	1	0.020

Probability of finding all units in energy state e_0: 0.391
Probability of finding two of three units in energy state e_0, and one of three units in energy state e_1: 0.431
WHY?

ANSWER:
The energy of the whole microstate is higher when one unit is in state e_1 and the other two are in e_0, so the probability of that state occurring is lower – ***BUT*** – that state occurs more often (*N = 3* vs. *N = 1*), so it becomes populated more often.

Microstates; Example 1 (7)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Exercise 1:

Select a different value for the energy at Level 1 (e_1).
(We had e_1 = 1 for the previous example.)
Figure out the set of probabilities for each of the microstates.
(You will have to compute a new value for Z.)

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Total Energy for that Microstate	$exp(-E_j)$ for that Microstate	*N = Total Accessible Microstate Instances*	$p_j = exp(-E_j) * N/Z$
1	3	0	0	1	1	?
2	2	1	1*x	?	3	?
3	1	2	2*x	?	3	?
4	0	3	3*x	?	1	?

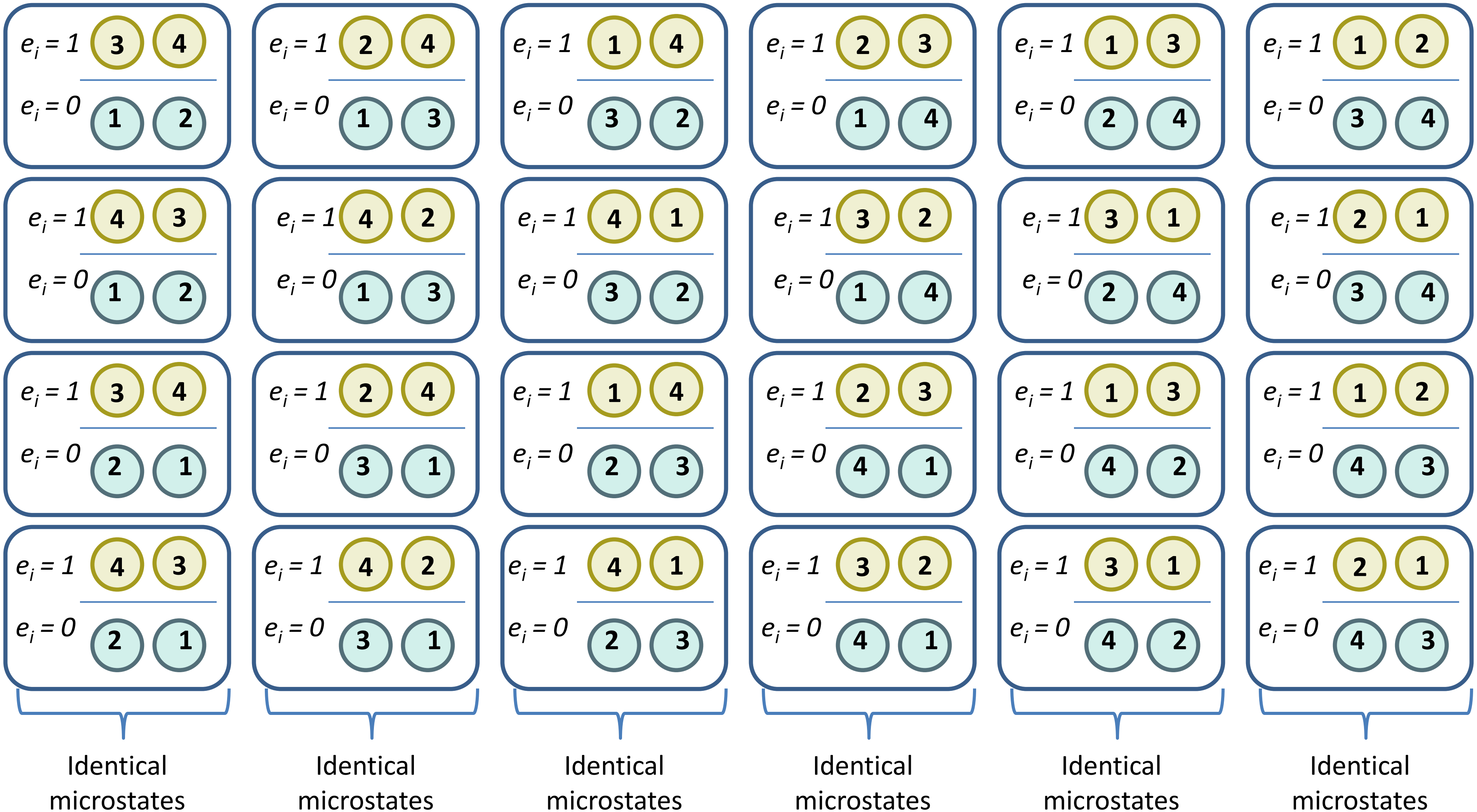
Interpret / explain your results.

Microstates : *Example 2* (1)

For a System with Four Units and Two Energy Levels;

Microstate Type: Two Units in Level $e_i = 0$, Two Units in Level $e_i = 1$

We can create 24 different nominal configurations, with SIX distinct (non-identical) microstates:



Microstates: *Example 2* (2)

We can create six different ***non-identical*** *configurations*

- Total ways of distributing the N units among the N different total spots: $N!$
  - Total number of spots available (same as total number of units): *4*
  - Choice of N different units to fill the first spot: Here, $N = 4$.
  - Choice of $N-1$ different (remaining) units to fill the next spot: Here, $N-1 = 3$.
  - Choice of $N-2$ different (remaining) units to fill the next spot: Here, $N-2 = 2$.
  - Total number of ways of distributing the $N = 4$ units: 4*3*2*1 = 24.
  - These 24 configurations contain *some which are identical* with the others.

- Number of units going into Level $e_i = 1$ (or e_1): 2
  - $N_1 = 2$; there are two spots at E_1; so we can have degeneracy at this level
  - The degeneracy is $N_1! = 2! = 2$.

- Number of ways of populating Level $e_j = 0$ (or e_0): 2
  - After we've put two of the units into Level e_1, there are $N_2 = N - N_1$ units left. (Here, $N_2 = 2$.)
  - The way in which we can multiply count the same configuration (the degeneracy) is $N_2! = 2! = 2$.

Number of *countably different* ways of populating the two states:

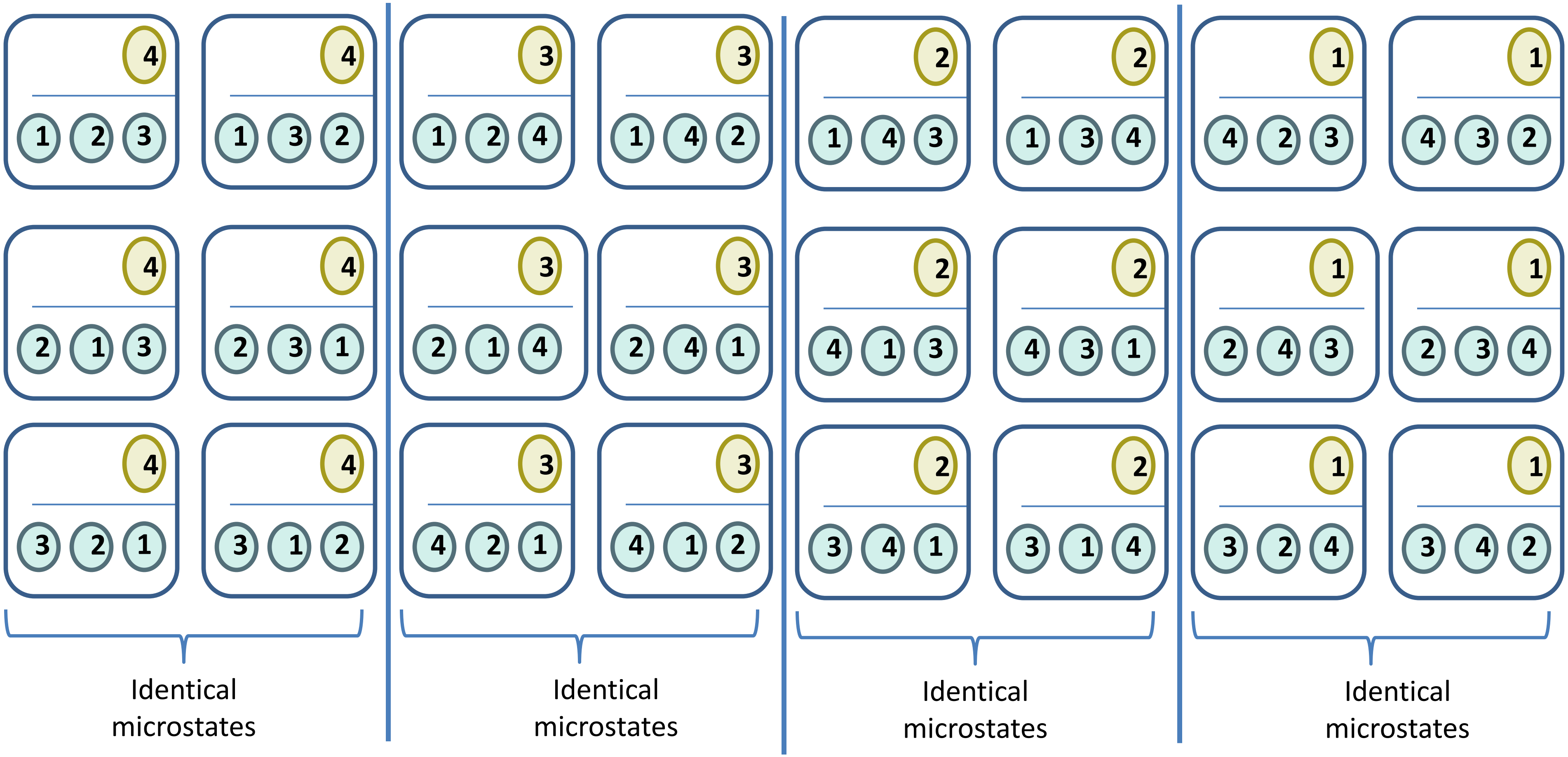
$$Z = \frac{N!}{N_1!N_2!} = \frac{4*3*2*1}{2!*2!} = \frac{24}{4} = 6$$

Microstates : *Example 2* (3)

For a System with Four Units and Two Energy Levels;

Microstate Type: Three Units in Level $e_i = 0$, One Unit in Level $e_i = 1$

We can create 24 different nominal configurations, with FOUR distinct (non-identical) microstates:



Microstates : *Example 2* (4)

For the Microstate Type: Three Units in Level $e_i = 0$, One Unit in Level $e_i = 1$
We can create four different ***non-identical*** *configurations*

- Total ways of distributing the N units among the N different total spots: $N!$
  - Total number of ways of distributing the $N = 4$ units: 4*3*2*1 = 24.
- Number of units going into Level $e_i = 1$ (or e_1): 1
  - N_1 = 1; there is one spot at e_1; so there is no degeneracy at this level.
  - The degeneracy is $N_1! = 1! = 1$.
- Number of ways of populating Level $e_i = 0$ (or e_0): 6 (with the remaining units)
  - After we've put one of the units into Level e_1 , there are $N_2 = N - N_1$ = 3 units left.
  - The way in which we can multiply count the same configuration (the degeneracy) is $N_2! = 3! = 3*2*1$.

Number of *countably different* ways of populating the two states:

$$Z = \frac{N!}{N_1!N_2!} = \frac{4*3*2*1}{3!*1!} = \frac{24}{(3*2*1)(1)} = 4$$

Microstates: Example 2 (5)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Computing the probability distribution

Example 2: Suppose that the energy of e_0 = 0, and the energy of e_1 = 1

$$p_j = \exp(-\beta E_j) / Z$$

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Energy for that Microstate	Total Energy for that Microstate	*exp(-E_j)* for that Microstate	*N = Total Accessible Microstate Instances*	*exp(-E_j) * N*
1	4	0	4*0 + 0*1	0	1	1	1.000
2	3	1	3*0 + 1*1	1	0.368	4	1.472
3	2	2	2*0 + 2*1	2	0.135	6	0.810
4	1	3	1*0 + 3*1	3	0.050	4	0.200
5	0	4	0*0 + 4*1	4	0.018	1	0.018

Sum of all the p_j*Z*N: 1.000 + 1.472 + 0.810 + 0.200 + 0.018 = 3.500

***Z* = 3.500**

Microstates; Example 2 (6)

Total Number of Accessible Microstates for an N = 3, 2-Level System

Computing the probability distribution

$$Z = \sum_j \exp(-\beta E_j)$$

Z = 3.500

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Total Energy for that Microstate	$exp(-E_j)$ for that Microstate	*N = Total Accessible Microstate Instances*	$p_j = exp(-E_j) * N/Z$
1	4	0	0	1	1	1.000/3.500 = 0.286
2	3	1	1	0.368	4	1.472/3.500 = 0.421
3	2	2	2	0.135	6	0.810/3.500 = 0.231
4	1	3	3	0.050	4	0.200/3.500 = 0.057
5	0	4	4	0.018	1	0.018/3.500 = 0.005

Sum of all p_j: 0.286 + 0.421 + 0.231 + 0.057 + 0.005 = 1.000

(Sum of the probabilities = 1)

Microstates; Example 2 (7)

Total Number of Accessible Microstates for an N = 4, 2-Level System

Exercise 2:

AS BEFORE: Select a different value for the energy at Level 1 (e_1).
(We had e_1 = 1 for the previous example.)
Figure out the set of probabilities for each of the microstates.
(You will have to compute a new value for Z.)

Microstate Type	Number of Units in Level e_0	Number of Units in Level e_1	Total Energy for that Microstate	$exp(-E_j)$ for that Microstate	*N = Total Accessible Microstate Instances*	$p_j = exp(-E_j) * N/Z$
1	4	0	0	1	1	?
2	3	1	1*x	?	4	?
3	2	2	2*x	?	6	?
4	1	3	3*x	?	4	?
5	0	4	4*x	?	1	?

Interpret / explain your results.