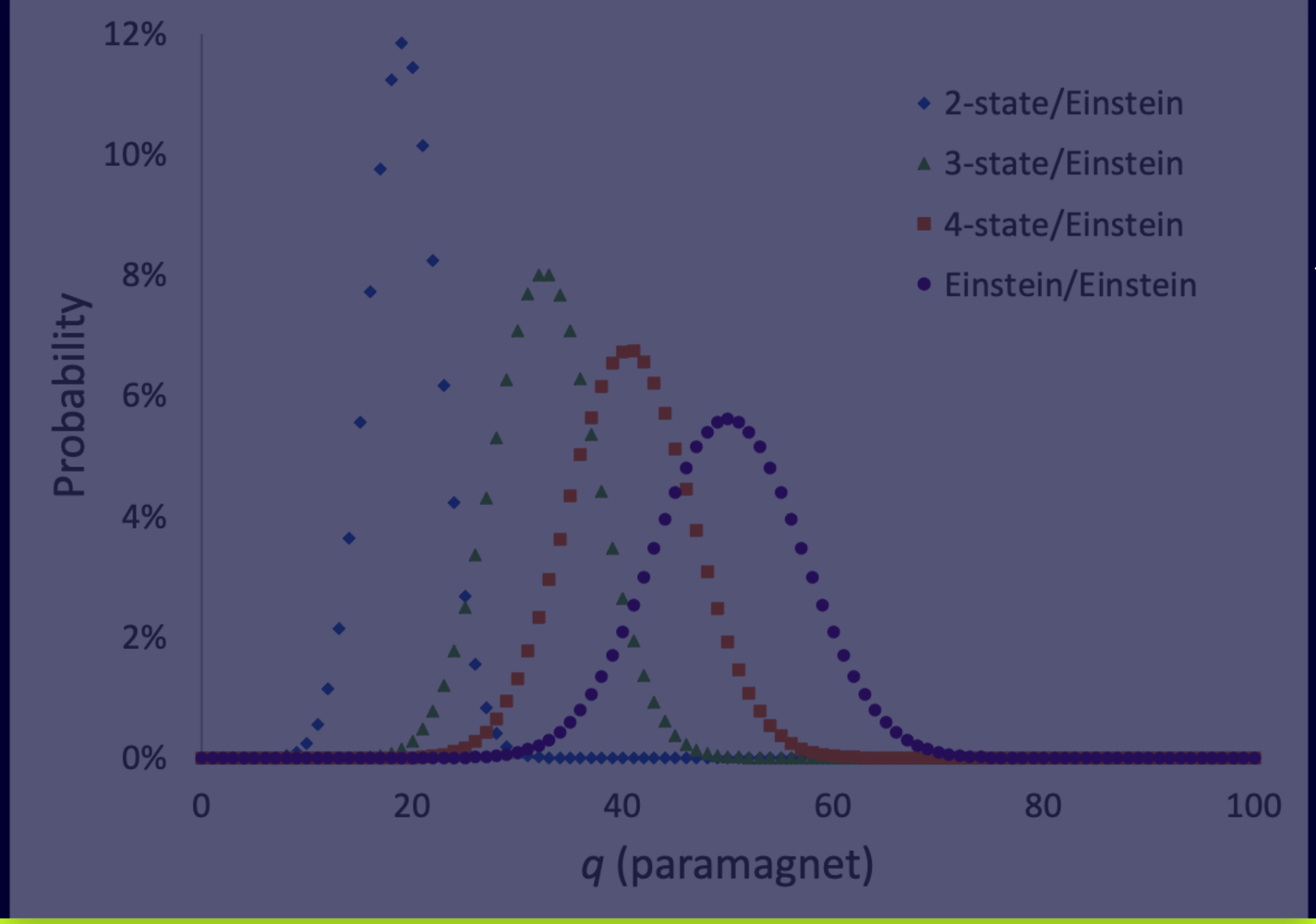
PICUP

ALMA COLLEGE



Counting microstates of the *p*-state paramagnet

DR. STEUARD JENSEN, ALMA COLLEGE

PICUP CAPSTONE CONFERENCE 12 AUG 2021

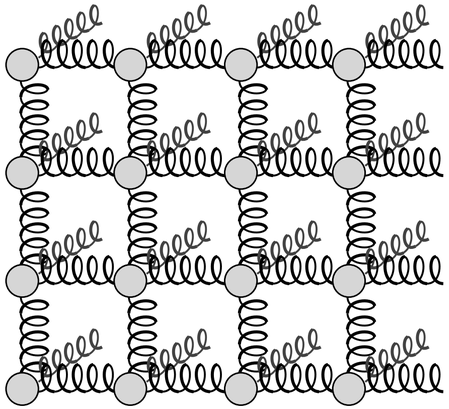
arXiv: 2108.10340

CHICKEN

No single definition of entropy simultaneously makes its meaning clear and the second law obvious.

	Meaning	Second Law
$dS = \frac{đQ}{T}$	“Disorder”??	$\frac{+đQ}{T_c} + \frac{-đQ}{T_h} > 0$ because $T_c < T_h$
$S = k \ln \Omega$	Counting microstates	Even though all microstates are equally likely, the macrostates with near-maximum entropy have enormously higher multiplicity, making it vanishingly improbable for systems to evolve to a lower-entropy state.

Moore & Schroeder (1997) proposed teaching irreversible behavior & the second law using computational state counting .



Einstein solid

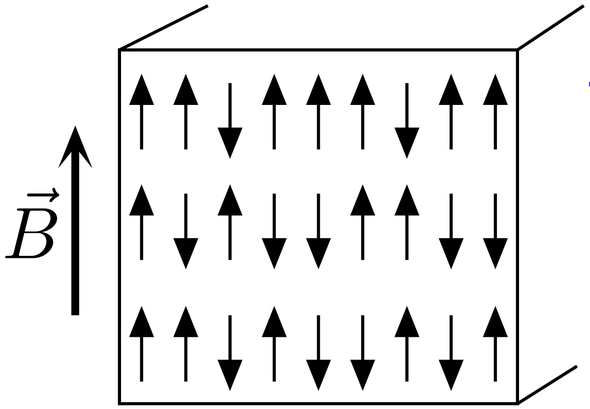
N oscillators from *N*/3 atoms

$3\hbar\omega$

$2\hbar\omega$

$\epsilon = \hbar\omega$

$0 = E_{\text{ground}}$



Two-state paramagnet

N spin-1/2 dipoles

$\epsilon = 2\mu B$

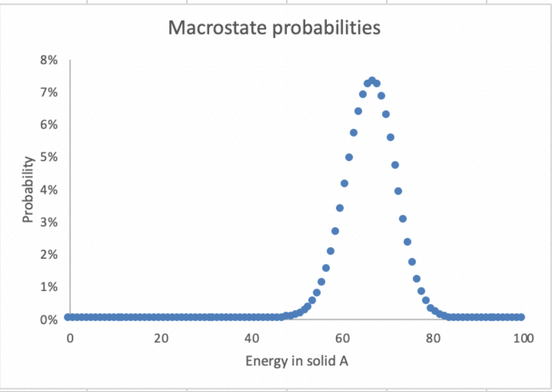
$0 = E_{\text{ground}}$

TwoEinSolids-2_10

Home Insert Draw Page Layout Formulas Data Review View

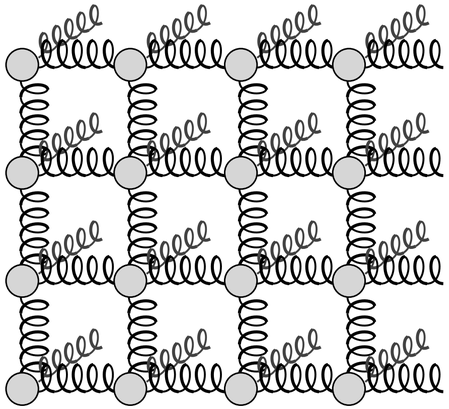
B9 =COMBIN(A9+B$3-1,A9)

	A	B	C	D	E	F
1	Two Einstein Solids					
2		N_total	300		Omega_all	1.68E+96
3	N_A	200	N_B	100	q	100
4						
5	q_A	Omega_A	q_B	Omega_B	Omega_tot	Probability
6	0	1.00E+00	100	4.53E+58	4.53E+58	2.69E-38
7	1	2.00E+02	99	2.28E+58	4.55E+60	2.71E-36
8	2	2.01E+04	98	1.14E+58	2.29E+62	1.36E-34
9	3	1.35E+06	97	5.66E+57	7.66E+63	4.55E-33
10	4	6.87E+07	96	2.80E+57	1.92E+65	1.14E-31
11	5	2.80E+09	95	1.38E+57	3.86E+66	2.30E-30
12	6	9.57E+10	94	6.75E+56	6.46E+67	3.84E-29
13	7	2.82E+12	93	3.29E+56	9.27E+68	5.51E-28
14	8	7.29E+13	92	1.59E+56	1.16E+70	6.91E-27
15	9	1.68E+15	91	7.67E+55	1.29E+71	7.69E-26
16	10	3.52E+16	90	3.67E+55	1.29E+72	7.70E-25
17	11	6.72E+17	89	1.75E+55	1.18E+73	7.00E-24
18	12	1.18E+19	88	8.28E+54	9.79E+73	5.82E-23
19	13	1.93E+20	87	3.90E+54	7.51E+74	4.47E-22
20	14	2.93E+21	86	1.82E+54	5.35E+75	3.18E-21
21	15	4.18E+22	85	8.48E+53	3.55E+76	2.11E-20
22	16	5.62E+23	84	3.92E+53	2.20E+77	1.31E-19
23	17	7.14E+24	83	1.80E+53	1.28E+78	7.64E-19
24	18	8.61E+25	82	8.20E+52	7.06E+78	4.20E-18
25	19	9.88E+26	81	3.71E+52	3.67E+79	2.18E-17
26	20	1.08E+28	80	1.67E+52	1.81E+80	1.08E-16
27	21	1.13E+29	79	7.47E+51	8.47E+80	5.04E-16
28	22	1.14E+30	78	3.31E+51	3.77E+81	2.24E-15
29	23	1.10E+31	77	1.46E+51	1.61E+82	9.55E-15
30	24	1.02E+32	76	6.39E+50	6.53E+82	3.88E-14
31	25	9.15E+32	75	2.78E+50	2.54E+83	1.51E-13



Moore & Schroeder: AJP (1997), arXiv:1502.07051

Students compute entropy by explicitly counting microstates for a fixed number q of equal-sized energy units: $q = U/\varepsilon$.

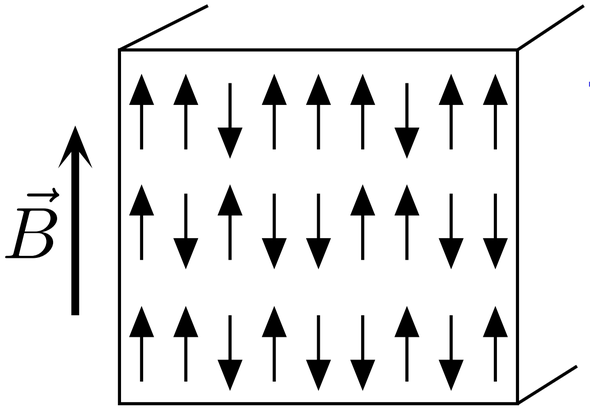


Einstein solid

N oscillators from $N/3$ atoms

$$\Omega = \binom{N+q-1}{q}$$

=COMBIN(N+q−1,q)

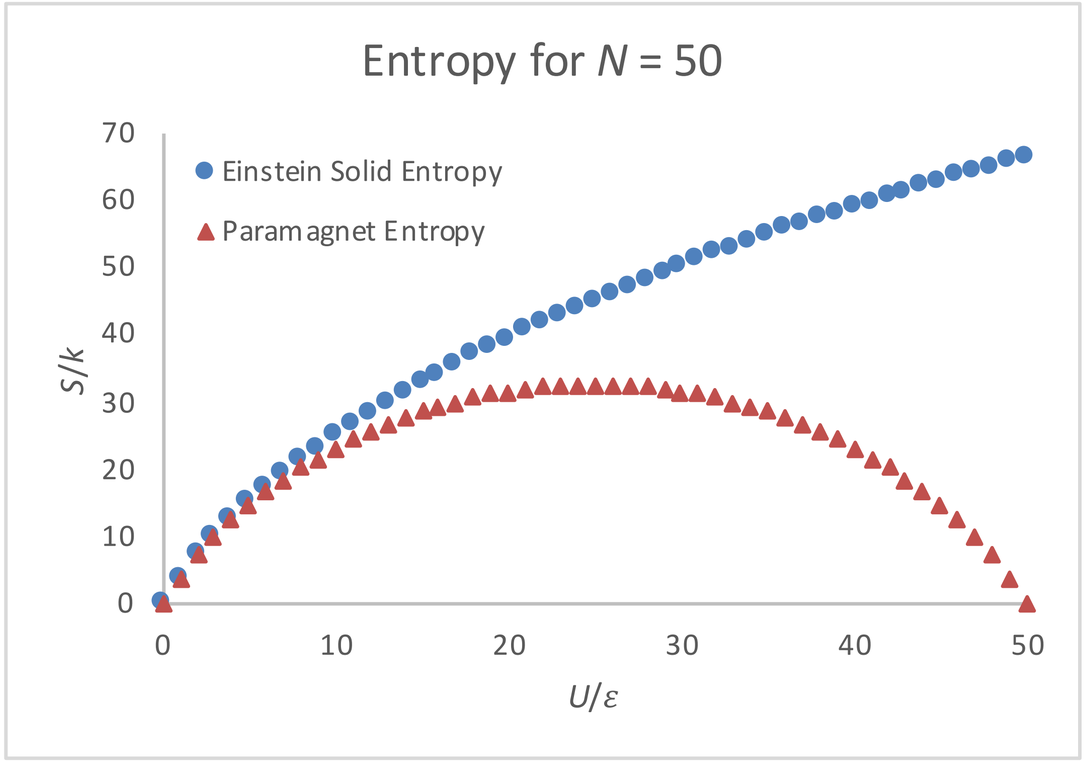


Two-state paramagnet

N spin-1/2 dipoles: $q = N_{\downarrow}$

$$\Omega = \binom{N}{q}$$

=COMBIN(N,q)

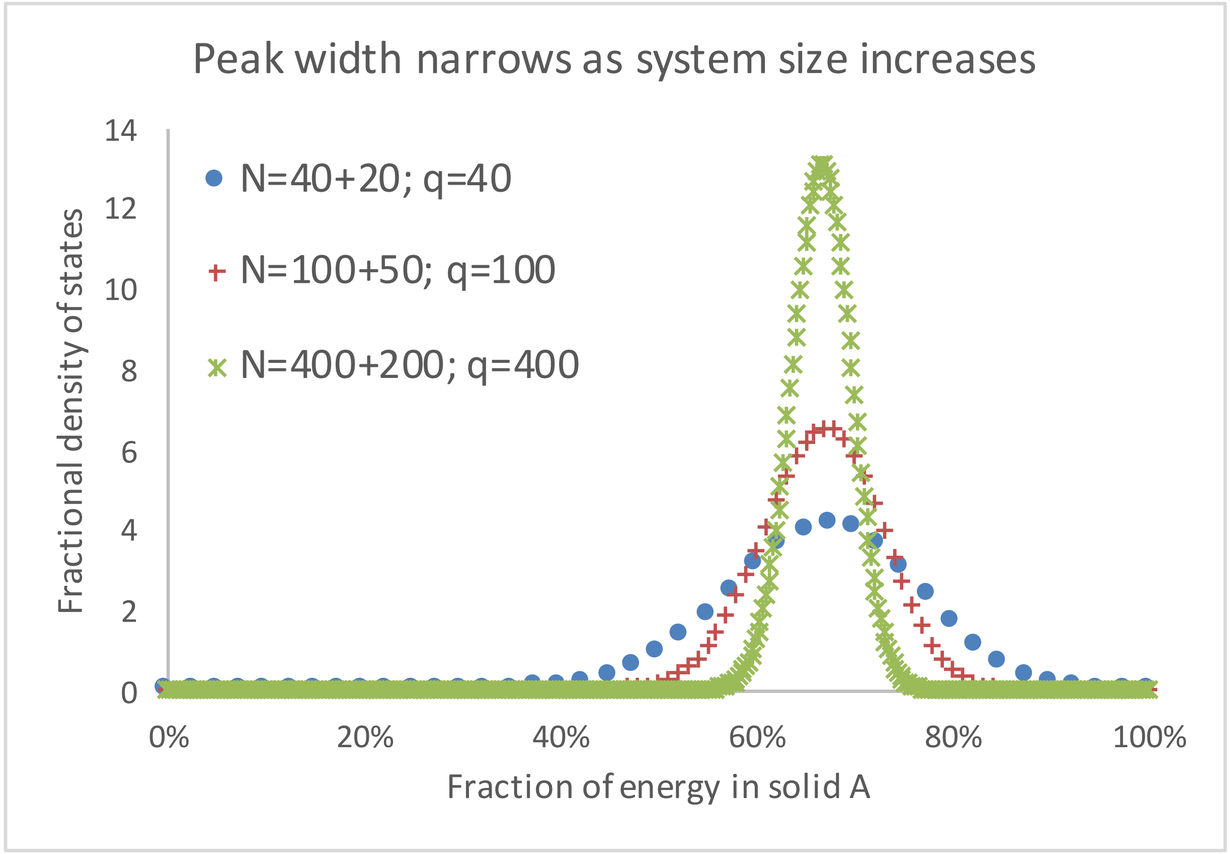


Students count states of interacting systems to discover that macrostates near maximum entropy are far more likely.

Specific student experiences:

(course using *Thermal Physics* by Schroeder)

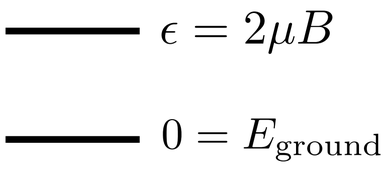
- Text shows interacting Einstein solids: how to compute multiplicities with a spreadsheet
- Students do that themselves, and adjust it to model interacting 2-state paramagnets
- Text shows how to compute the heat capacity for 2-state paramagnet
- Students use a spreadsheet to compute heat capacity for an Einstein solid



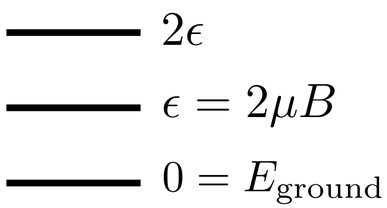
A weak point: After all this investment in computational methods, there's nothing else to do!

State counting for a paramagnet of arbitrary spin is more complicated, but still manageable.

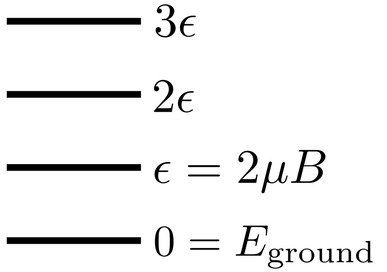
2-state: $J = 1/2$



3-state: $J = 1$



4-state: $J = 3/2$



For N dipoles with q units of energy, count states using *extended binomial coefficients*:

$$\Omega = \binom{N}{q} = \binom{N}{q}^{\{1\}}$$

Coefficient of x^q in . . .
$(1+x)^N$

$$\Omega = \binom{N}{q}^{\{2\}}$$

Coefficient of x^q in . . .
$(1+x+x^2)^N$

$$\Omega = \binom{N}{q}^{\{3\}}$$

Coefficient of x^q in . . .
$(1+x+x^2+x^3)^N$

S. Jensen: arXiv:2108.10340 (submitted to AJP)

Computing these multiplicities is difficult in a spreadsheet, so the instructor may want to provide that data to students.

$$\Omega = \binom{N}{q}^{\{p-1\}} = \sum_{j=0}^{\lfloor q/p \rfloor} (-1)^j \binom{N}{j} \binom{N+q-pj-1}{q-pj}$$

N	p	$q=0$	1	2	3	4	5	6	7	8	9
3	2	1	3	3	1	0	0	0	0	0	0
3	3	1	3	6	7	6	3	1	0	0	0
3	4	1	3	6	10	12	12	10	6	3	1
3	∞	1	3	6	10	15	21	28	36	45	55
6	2	1	6	15	20	15	6	1	0	0	0
6	3	1	6	21	50	90	126	141	126	90	50
6	4	1	6	21	56	120	216	336	456	546	580
6	∞	1	6	21	56	126	252	462	792	1287	2002

$$\binom{N}{q}^{\{\infty\}} \equiv \binom{N+q-1}{q} \quad \text{(Einstein solid)}$$

Mathematica:

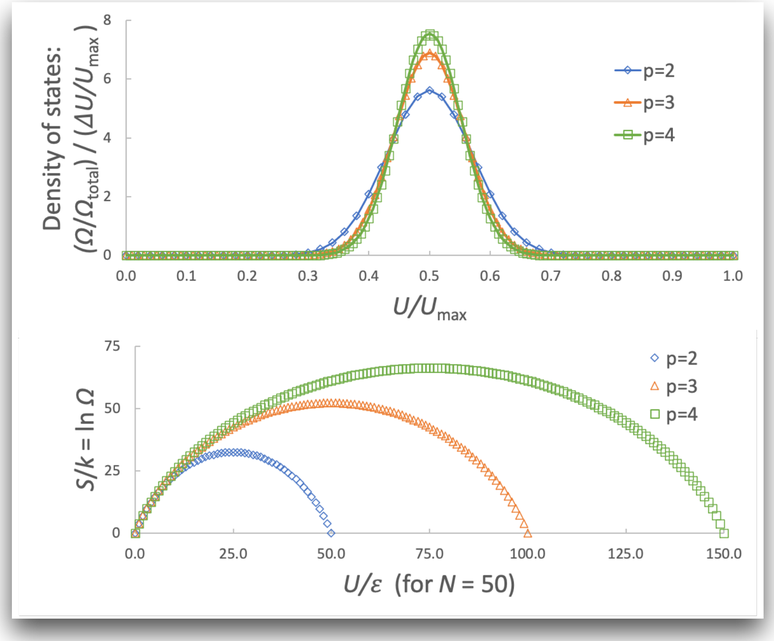
```
Coefficient[Sum[x^a, {a, 0, p-1}]^n, x, q]
```

Python:

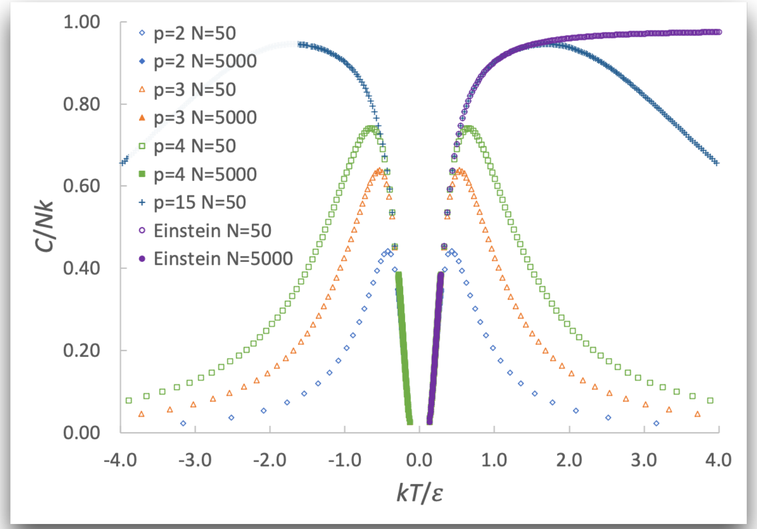
```
import scipy.special as sp
def extBinom(n,q,p,exact=True):
  result = 0
  for j in range(q//p + 1):
    result += (-1)**j * sp.comb(n,j,exact) \
        * sp.comb(n+q-p*j-1,q-p*j,exact)
  return result
```

Given this multiplicity data, students can explore patterns in entropy, heat capacity, interactions, and more.

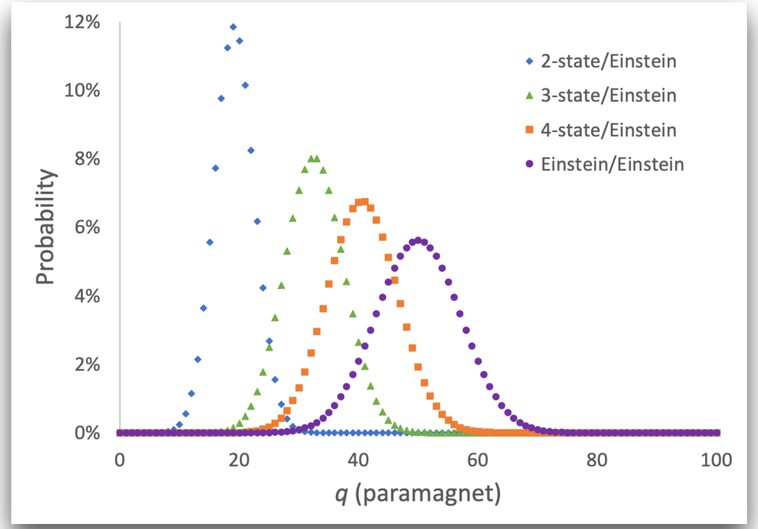
State counting and entropy



Heat capacity vs. temperature

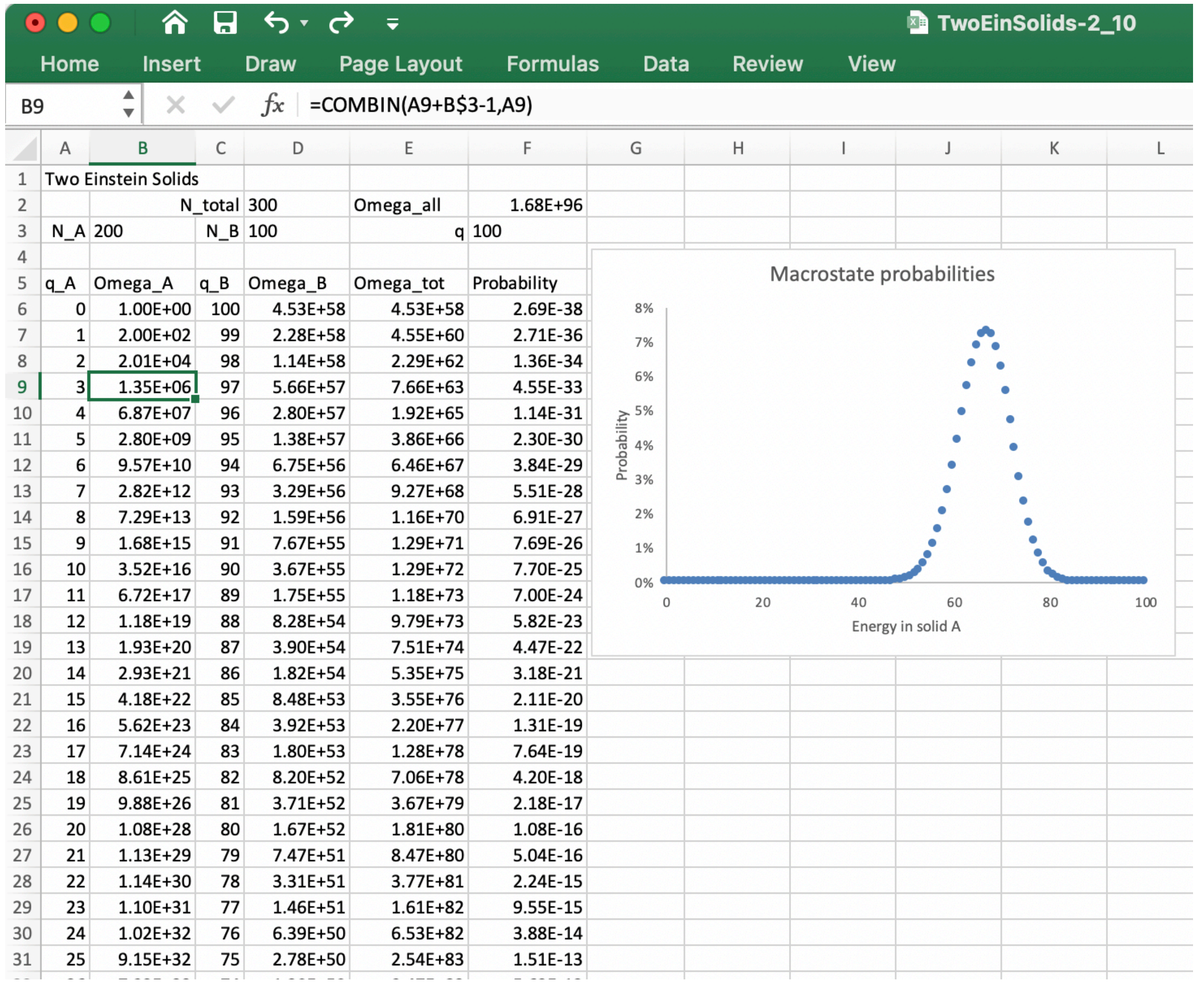


Interactions with Einstein solid



Take-home messages:

- Spreadsheets are an effective tool for teaching students about entropy.
- General *p*-state paramagnet systems provide a wide range of examples and questions to explore, expanding the computational opportunities in the course.
- (Analytic analysis is also possible, though only in certain limits.)



	A	B	C	D	E	F
1	Two Einstein Solids					
2		N_total	300	Omega_all		1.68E+96
3	N_A	200	N_B	100	q	100
4						
5	q_A	Omega_A	q_B	Omega_B	Omega_tot	Probability
6	0	1.00E+00	100	4.53E+58	4.53E+58	2.69E-38
7	1	2.00E+02	99	2.28E+58	4.55E+60	2.71E-36
8	2	2.01E+04	98	1.14E+58	2.29E+62	1.36E-34
9	3	1.35E+06	97	5.66E+57	7.66E+63	4.55E-33
10	4	6.87E+07	96	2.80E+57	1.92E+65	1.14E-31
11	5	2.80E+09	95	1.38E+57	3.86E+66	2.30E-30
12	6	9.57E+10	94	6.75E+56	6.46E+67	3.84E-29
13	7	2.82E+12	93	3.29E+56	9.27E+68	5.51E-28
14	8	7.29E+13	92	1.59E+56	1.16E+70	6.91E-27
15	9	1.68E+15	91	7.67E+55	1.29E+71	7.69E-26
16	10	3.52E+16	90	3.67E+55	1.29E+72	7.70E-25
17	11	6.72E+17	89	1.75E+55	1.18E+73	7.00E-24
18	12	1.18E+19	88	8.28E+54	9.79E+73	5.82E-23
19	13	1.93E+20	87	3.90E+54	7.51E+74	4.47E-22
20	14	2.93E+21	86	1.82E+54	5.35E+75	3.18E-21
21	15	4.18E+22	85	8.48E+53	3.55E+76	2.11E-20
22	16	5.62E+23	84	3.92E+53	2.20E+77	1.31E-19
23	17	7.14E+24	83	1.80E+53	1.28E+78	7.64E-19
24	18	8.61E+25	82	8.20E+52	7.06E+78	4.20E-18
25	19	9.88E+26	81	3.71E+52	3.67E+79	2.18E-17
26	20	1.08E+28	80	1.67E+52	1.81E+80	1.08E-16
27	21	1.13E+29	79	7.47E+51	8.47E+80	5.04E-16
28	22	1.14E+30	78	3.31E+51	3.77E+81	2.24E-15
29	23	1.10E+31	77	1.46E+51	1.61E+82	9.55E-15
30	24	1.02E+32	76	6.39E+50	6.53E+82	3.88E-14
31	25	9.15E+32	75	2.78E+50	2.54E+83	1.51E-13