Statistical Interactions I: Combinatorics [tsc20]

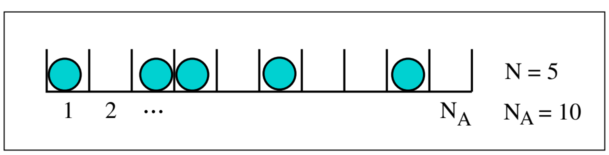
The term *statistical interaction* covers a lot of ground.

- Multiple occupancy of 1-particle states is permitted for bosons and prohibited for fermions. The exclusion principle is a statistical interaction.
- Phonons are collective excitations representing atomic vibrations in solids. Their statistical interaction is encoded in the bosonic statistics and the band structure.
- Conduction electrons in metals are represented by collective excitations whose statistical interaction is encoded in the fermionic statistics and the band structure.
- Most steric interactions (e.g. hard-core repulsions) simply involve excluded volumes and thus become statistical interactions. No interaction energies are in play.
- Statistical interactions are easier to cope with than dynamical interactions. Interaction energies between simple particles become activation energies of more complex particles.

This module offers a gentle introduction to the combinatorics of statistically interacting particles. Particle energies have no part in this aspect.

Fermions:

Consider a system with N_A orbitals and N particles. Orbitals are distinguishable. Particles are indistinguishable. Multiple occupancy is prohibited (a manifestation of the Pauli principle).



Binomial expression for the number of distinct microstates with N particles:

$$W(N) = \binom{N_A}{N} = \frac{N_A!}{N!(N_A - N)!}\,.$$

Multiplicity expression in standardized form (for one species):

$$W(N) = \binom{d + N - 1}{N}, \quad d = A - g(N-1), \quad A = N_A, \quad g = 1.$$

A: number of options available for placing the first particle into the array of orbitals (capacity constant).

g: impact of placing one particle on the capacity of placing further particles into the orbitals (statistical interaction coefficient).

d: number of options for placing $N^{\rm th}$ particle with $N-1$ already placed.

The maximum capacity is reached when $N = N_A$: $W(N_A + 1) = 0$.

Representation of fermionic microstates for $N_A = 4$ and $N = 0, 1, 2, 3, 4$:

0000
1000 0100 0010 0001
1100 1010 1001 0110 0101 0011
1110 1101 1011 0111
1111

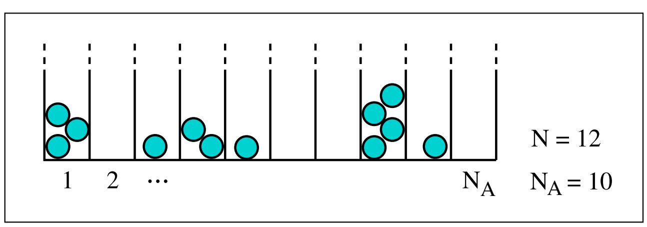
Placing one fermion, $\Delta N = 1$, reduces the options for placing next the fermion as follows: $\Delta d = -\Delta N = -1$.

Placing the $N^{\rm th}$ fermion for $N_A = 4$ (with $N-1$ fermions already in place):

$N = 1 \quad \Rightarrow \quad d = 4$: 0000 $\rightarrow$ 1000 0100 0010 0001
$N = 2 \quad \Rightarrow \quad d = 3$: 1000 $\rightarrow$ 1100 1010 1001
$N = 3 \quad \Rightarrow \quad d = 2$: 1100 $\rightarrow$ 1110 1101
$N = 4 \quad \Rightarrow \quad d = 1$: 1110 $\rightarrow$ 1111
$N = 5 \quad \Rightarrow \quad d = 0$

Bosons:

Consider a system with N_A orbitals and N bosonic particles. Orbitals are distinguishable. Particles are indistinguishable. Multiple occupancy is permitted and unrestricted.



Binomial expression for the number of distinct microstates with N particles:

$$W(N) = \begin{pmatrix} N_A + N - 1 \\ N \end{pmatrix} = \frac{(N_A + N - 1)!}{N!(N_A - 1)!} \, .$$

Multiplicity expression in standardized form previously used for fermions:

$$W(N) = \binom{d+N-1}{N}, \quad d = A - g(N-1), \quad A = N_A, \quad g = 0.$$

The system has unlimited capacity for populating oribitals with bosons.

Representation of bosonic microstates for $N_A = 3$ and $N = 0, 1, 2, 3$:

000
100 010 001
200 020 002 110 101 011
300 030 003 120 102 012 210 201 021 111

Placing a boson does not reduce options for placing next boson: $\Delta d = 0$.
Three cases of placing N^{th} boson for $N_A = 3$:

$N = 1 \quad \Rightarrow \; d = 3$: 000 $\rightarrow$ 100 010 001
$N = 2 \quad \Rightarrow \; d = 3$: 100 $\rightarrow$ 200 110 101
$N = 3 \quad \Rightarrow \; d = 3$: 110 $\rightarrow$ 210 120 111

An alternative (fermionic looking) binomial expression for bosonic combinatorics introduces N_B effective orbitals with multiple occupancy prohibited:

$$W(N) = \binom{N_B}{N}, \quad N_B = N_A + N - 1.$$

Bosonic microstates for $N_A = 2$, i.e. $N_B = 2 + N$ and $N = 0, 1, 2, 3$ in the alternative representation:

00
100 010 001
1100 1010 1001 0110 0101 0011
11100 11010 11001 10110 10101 10011 01110 01101 01011 00111

This representation turns out to be more useful for the purpose of generalizations to less familiar statistics.

Size L and XL particles:

Place N (indistinguishable) particles into an array of N_A (distinguishable) orbitals. We provisionally assume that the array is linear.

Any two particles must be at least g sites apart. This covers the cases $g = 1$ (fermions) and $g = 0$ (bosons) discussed previously.

– Capacity constant: $A = N_A$.
– Statistical interaction coefficients:[1] $g = 0, 1, 2, \ldots$
– Generalized Pauli principle: $d = A - g(N - 1)$.

Multiplicity expression in standardized form:

$$W(N) = \begin{pmatrix} d + N - 1 \\ N \end{pmatrix} = \frac{(d + N - 1)!}{N!(d - 1)!}.$$

Microstates of particles with $g = 2$ for $N_A = 5$ and $N = 0, 1, 2, 3$:

00000
10000 01000 00100 00010 00001
10100 10010 10001 01010 01001 00101
10101

Between any two occupied orbitals, there is at least one vacant orbital.

The alternative representation of microstates introduces N_B effective orbitals with multiple occupancy prohibited and no need for extra space.

$$W(N) = \begin{pmatrix} N_B \\ N \end{pmatrix}, \quad N_B = A - (g - 1)(N - 1).$$

Equivalent microstates for $N_B = 6 - N$ and $N = 0, 1, 2, 3$:

000000
10000 01000 00100 00010 00001
1100 1010 1001 0110 0101 0011
111

This representation does not require the array to be linear. It is the one that naturally extends to cases of fractional statistics.

Semions:

Place N (indistinguishable) semionic particles into an array of N_A (distinguishable) orbitals. The placement of one particle reduces the options for placing further particles by one half.[2]

[1] In the airline industry $g = 0, 1, 2, 3$ might stand for cargo, economy, business, first class.
[2] Haldane 1991.

– Statistical interaction coefficient: $g = \frac{1}{2}$ (fractional statistics).

– Capacity constant: $A = \begin{cases} N_A & \text{for } N = 1, 3, 5, \ldots \\ N_A + \frac{1}{2} & \text{for } N = 0, 2, 4, \ldots \end{cases}$

Multiplicity expression in standardized form:

$$W(N) = \binom{d + N - 1}{N}, \quad d = A - g(N - 1).$$

Multiplicity expression which uses effective fermionic orbitals:

$$W(N) = \binom{N_B}{N}, \quad N_B = A - (g - 1)(N - 1).$$

Microstates of particles for $N_A = 3$ has varying $N_B = A + \frac{1}{2}(N - 1)$:

$N = 0, 2, 4, 6$	$N = 1, 3, 5$
000	100 010 001
1100 1010 1001 0110 0101 0011	1110 1101 1011 0111
11110 11101 11011 10111 01111	11111
111111	

In this representation placing two semions goes along with adding one orbital.

Prominent applications of semionic statistics include spinon excitations in quantum spin chains and antiferromagnetic domain walls in Ising chains.

Orbitals that permit up to double occupancy are not semionic in nature. Multiple occupancy is often associated with internal degrees of freedom.

Particles with internal degrees of freedom:

Internal degrees of freedom are distinguishable traits of otherwise indistinguishable particles. e.g. electrons (fermions) with spin $\uparrow$ or $\downarrow$.

Microstates for $N_A = 2$ orbitals and $N = 0, 1, \ldots, 4$ electrons
(0: vacancy; $\uparrow, \downarrow$: single occupancy; $\updownarrow$: double occupancy):

00	(00)(00)
$\uparrow$0 0$\uparrow$ $\downarrow$0 0$\downarrow$	($\uparrow$0)(00) (0$\uparrow$)(00) (00)($\downarrow$0) (00)(0$\downarrow$)
$\updownarrow$0 0$\updownarrow$ $\uparrow\downarrow$ $\downarrow\uparrow$ $\uparrow\uparrow$ $\downarrow\downarrow$	($\uparrow$0)($\downarrow$0) (0$\uparrow$)(0$\downarrow$) ($\uparrow$0)(0$\downarrow$) (0$\uparrow$)($\downarrow$0) ($\uparrow\uparrow$)(00) (00)($\downarrow\downarrow$)
$\updownarrow\uparrow$ $\updownarrow\downarrow$ $\uparrow\updownarrow$ $\downarrow\updownarrow$	($\uparrow\uparrow$)($\downarrow$0) ($\uparrow$0)($\downarrow\downarrow$) ($\uparrow\uparrow$)(0$\downarrow$) (0$\uparrow$)($\downarrow\downarrow$)
$\updownarrow\updownarrow$	($\uparrow\uparrow$)($\downarrow\downarrow$)

An alternative representation of the same microstates is shown on the right.

Consider, more generally, a system of particles with a two-valued internal degree of freedom and exclusion statistics $g \geq 0$ occupying N_A orbitals.

We effectively have two sets of orbitals and two species of particles. The multiplicity expression (in standardized form) factorizes:

$$W(N_1, N_2) = \left(\begin{array}{c} d_1 + N_1 - 1 \\ N_1 \end{array} \right) \left(\begin{array}{c} d_2 + N_2 - 1 \\ N_2 \end{array} \right),$$

$$d_1 = A_1 - g(N_1 - 1), \qquad d_2 = A_1 - g(N_2 - 1).$$

If all distinguishable traits of the internal degree of freedom are ignorable, we can effectively merge the two species of particles:

$$W(N) = \sum_{N_1=0}^{N} W(N_1, N - N_1) = W(N) = \left(\begin{array}{c} d + N - 1 \\ N \end{array} \right).$$

$$d = A - g(N - 1), \quad N = N_1 + N_2, \quad A = A_1 + A_2.$$

In the representation on the right of the example shown, the merger ignores the distinction between $\uparrow$ and $\downarrow$. The number of microstates does not change.

For a comparison with the situation discussed next, we rewrite the multiplicity expression for distinguishable particles in separate orbitals as follows:

$$W(N_1, N_2) = \left(\begin{array}{c} d_1 + N_1 - 1 \\ N_1 \end{array} \right) \left(\begin{array}{c} d_2 + N_2 - 1 \\ N_2 \end{array} \right),$$

$$d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}), \quad \mathbf{g} = \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right), \quad A_1 + A_2 = N_A.$$

It is convenient to write the statistical interaction coefficients as elements of a matrix (or tensor) and to generalize the expression for d_m as shown.

Distinguishable species particles in shared orbitals:

Consider a system of N_A orbitals. Each orbital is either vacant or populated by one particle from species 1 or species 2.

The standardized multiplicity expression now involves off-diagnonal elements of $\mathbf{g}$, indicative of an inter-species statistical interaction:[3]

$$W(N_1, N_2) = \left(\begin{array}{c} d_1 + N_1 - 1 \\ N_1 \end{array} \right) \left(\begin{array}{c} d_2 + N_2 - 1 \\ N_2 \end{array} \right),$$

$$d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}), \quad \mathbf{g} = \left(\begin{array}{cc} 1 & 1 \\ 0 & 1 \end{array} \right), \quad A_1 = A_2 = N_A.$$

[3]Interchanging the values of g_{12} and g_{21} yields the same function $W(N_1, N_2)$.

Microstates for $N_A = 2$ and $N_A = 3$:

00	000
10 01, 20 02	100 010 001, 200 020 002
11, 22, 12 21	110 101 011, 220 202 022, 120 102 012, 210 201 021
	111, 222, 112 121 211, 122 212 221

The two species are not mergeable if they share orbitals. Removing or ignoring distinguishable particle traits changes the number of microstates.

Variations and extensions:

- If M species of particles are present, $W(N_1, \ldots, N_M)$ has M binomial factors and the matrix $\mathbf{g}$ grows to size $M \times M$ with zeros below the diagonal and ones elsewhere.
- If multiple occupancy of orbitals without limit is permitted, we must use $g_{mm'} = 0$ instead.
- If particles of either species must be spaced g cells apart, we must use $g_{11} = g_{12} = g_{22} = g$ and $g_{21} = g - 1$.

Particle species discussed thus far are categorized as compacts. The sequence in which compacts are placed into an orbital (if allowed) does not matter.

Hosts and caps:

Consider a system of N_A orbitals. Each orbital may be vacant, singly occupied, or doubly occupied by particles of a single species.

In this case, the rank in placement (first or second) counts as a distinguishable trait even if the particles are otherwise identical. The first particle placed into an orbital is named host and the second particle placed is named cap.

Multiplicity of microstates with N_1 hosts and N_2 caps:

$$W(N_1, N_2) = \left(\begin{array}{c} d_1 + N_1 - 1 \\ N_1 \end{array} \right) \left(\begin{array}{c} d_2 + N_2 - 1 \\ N_2 \end{array} \right),$$

$$d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}),$$

$$\mathbf{g} = \left(\begin{array}{cc} 1 & 0 \\ -1 & 1 \end{array} \right), \quad A_1 = N_A, \quad A_2 = 0.$$

- The reference state (all orbitals vacant) has capacity for placing a host in N_A slots ($A_1 = N_A$), but no capacity for placing a cap ($A_2 = 0$).

- Adding a host decreases the capacity for placing further hosts ($g_{11} = 1$), but increases the capacity for placing caps ($g_{21} = -1$).
- Adding a cap does not affect the capacity for placing hosts ($g_{12} = 0$) but decreases the capacity for placing further caps ($g_{22} = 1$).

Microstates for $N_A = 2$ and $N_A = 3$: [0: vacancy, 1: host, 2: host & cap]

	000
00	100 010 001
10 01	110 101 011, 200 020 002
20 02, 11	111, 210 201 021 120 102 012
21 12	211 121 112, 220 202 022
22	221 212 122
	222

The total number of microstates generated by hosts and caps in N_A orbitals is N_A^3, equal to that of two species of fermionic compacts with distinguishable traits (previous section), but distributed differently.

Hosts and caps are a case of nested particles. Caps can only be placed (metaphoriclly) on top of hosts which already in the orbitals.

Hosts, hybrids, and caps:

We generalize the host/cap situation from orbitals that permit double occupancy to orbitals that allow a maximum occupancy of $3 \leq M < \infty$.

- The first particle placed into an orbital belongs to the host category.
- The next $M-2$ particles placed in the same orbital have the capability of hosting and being hosted. They are categorized as hybrids.
- The (last) M^{th} particle that fits into the orbital is a cap.

The multiplicity of microstates for the case $M = 3$ with N_1 hosts, N_2 hybrids, and N_3 caps in the standardized format is,

$$W(\{N_m\}) = \prod_{m=1}^{3} \binom{d_m + N_m - 1}{N_m}, \quad d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}),$$

$$\mathbf{g} = \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}, \quad A_1 = N_A, \quad A_2 = A_3 = 0.$$

- Adding a particle of any species decreases the capacity for placing further particles of the same species ($g_{11} = g_{22} = g_{33} = 1$).

– Adding a host opens a slot for a hybrid ($g_{21} = -1$).

– Likewise, adding a hybrid opens a slot for a cap ($g_{32} = -1$).

– Any instance of $g_{mm'} = 0$ means that the available slots for particle species m is unaffected when a particle of species m' is placed.

Microstates for $N_A = 2$ and $N_A = 3$:
[0: vacancy, 1: host, 2: host & hybrid, 3: host & hybrid & cap]

	000
	100 010 001
00	110 101 011, 200 020 002
10 01	111, 210 201 021 120 102 012, 300 030 003
20 02, 11	211 121 112, 220 202 022, 310 301 031 130 103 013
30 03, 21 12	221 212 122, 311 131 113, 320 302 032 230 203 023
31 13, 22	222, 321 213 132 312 123 231, 330 303 033
32 23	322 232 223, 331 313 133
33	332 323 233
	333

In the general case, the matrix $\mathbf{g}$ is of size $M \times M$ with nonzero elements $g_{mm} = 1$ on the diagonal and $g_{m,m-1} = -1$ just below the diagonal.

Hosts, hybrids, and tags:

Consider a system of N_A orbitals, which may be vacant or occupied by any number of particles. The rank in placement is potentially a distinguishable trait for particles. In the absence of any such trait we are dealing with bosons.

If only the first particle in an orbital has a distinctive trait, we have a system of hosts and tags. One host precedes any number of tags in an orbital.

Multiplicity of microstates with N_1 hosts and N_2 tags (across all orbitals):

$$W(N_1, N_2) = \left(\begin{array}{c} d_1 + N_1 - 1 \\ N_1 \end{array} \right) \left(\begin{array}{c} d_2 + N_2 - 1 \\ N_2 \end{array} \right),$$

$$d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}),$$

$$\mathbf{g} = \left(\begin{array}{cc} 1 & 0 \\ -1 & 0 \end{array} \right), \quad A_1 = N_A, \quad A_2 = 0.$$

– The system without particles has only capacity for hosts ($A_1 = N_A$), not for tags ($A_2 = 0$).

– Adding hosts decreases capacity for further hosts ($g_{11} = 1$), but increases capacity for tags ($g_{21} = -1$).

– Adding tags does not affect capacity for hosts ($g_{12} = 0$) or for further tags ($g_{22} = 0$).

If we also assign a distinguishable trait to the particles placed second in an orbital we have a system hosts, hybrids, and tags.

Multiplicity of microstates with N_1 hosts, N_2 hybrids, and N_3 tags :

$$W(\{N_m\}) = \prod_{m=1}^{3} \left(\begin{array}{c} d_m + N_m - 1 \\ N_m \end{array} \right), \quad d_m = A_m - \sum_{m'} g_{mm'}(N_{m'} - \delta_{mm'}),$$

$$\mathbf{g} = \left(\begin{array}{rrr} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & -1 & 0 \end{array} \right), \quad A_1 = N_A, \quad A_2 = A_3 = 0.$$

– The key difference between caps and tags is that caps close down slots ($g_{\rm cc} = 1$), whereas tags leave them open ($g_{\rm tt} = 0$).

– The role of hybrids is the same in combination with tags and caps.

– The nesting can be extended to $M-2$ hybrids. The matrix $\mathbf{g}$ is of size $M \times M$ with nonzero elements $g_{mm} = 1$ on the diagonal for $m < M$ and $g_{m,m-1} = -1$ just below the diagonal.

Microstates for $M = 3$ (one hybrid species):
[0: vacancy, 1: host, 2: host & hybrid, $n \geq 3$: host & hybrid & $n-2$ tags]

$N_A = 2$ and $N_1 + N_2 + N_3 \leq 5$ and $N_A = 3$ and $N_1 + N_2 + N_3 \leq 5$:

00
10 01
20 02, 11
30 03, 21 12
40 04, 31 13, 22
50 05, 41 14, 32 23

000
100 010 001
200 020 002, 110 101 011
300 030, 003, 210 201 021 120 102 012, 111
400 040 004, 220 202 022, 310 103 031 130 301 013, 211 121 112
500 050 005, 410 104 041 140 401 014, 230 302 023 320 203 032,
221 212 122, 311 131 113

Configurational entropy:

The natural logarithm of the multiplicity $W(\{N_m\})$ of microstates with given numbers of particles, $\{N_m\}$, is a configurational entropy in the restricted sense that all microstates have equal probability. The expression [tex186],

$$S(\{N_m\}) = k_\mathrm{B} \ln\big(W(\{N_m\})\big) = k_\mathrm{B} \sum_m \Big[\big(N_m + Y_m\big)\ln\big(N_m + Y_m\big) - N_m \ln N_m - Y_m \ln Y_m\Big],$$

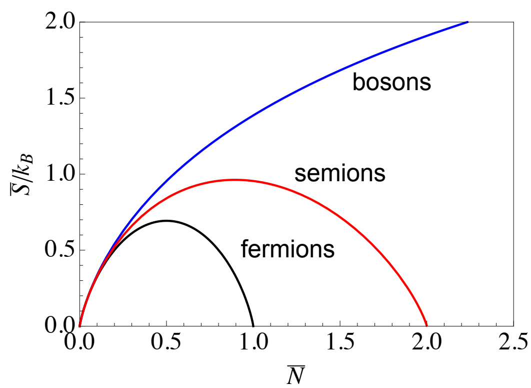
$$Y_m = A_m - \sum_{m'} g_{mm'} N_{m'}$$

is exact for a macroscopic system.[4] It depends on the capacity constants A_m, the statistical interaction coefficients $g_{mm'}$, and the particle content $\{N_m\}$.

The extensivity of the entropy is encoded in the capacity constants A_m of compacts and/or hosts.

Examples with one species of particles.

We compare the entropy per orbital, $\bar{S} \doteq S/N_A$, as a function of the population density, $\bar{N} \doteq N/N_A$, in the limit $N_A \to \infty$ for fermions ($g = 1$), bosons ($g = 0$), and semions ($g = \frac{1}{2}$).



$$\bar{S}/k_\mathrm{B} = -\big(1-\bar{N}\big)\ln\big(1-\bar{N}\big) - \bar{N}\ln\bar{N} \quad : \ g = 1,$$

$$\bar{S}/k_\mathrm{B} = \big(1+\bar{N}\big)\ln\big(1+\bar{N}\big) - \bar{N}\ln\bar{N} \quad : \ g = 0,$$

$$\bar{S}/k_\mathrm{B} = \big(1+\tfrac{1}{2}\bar{N}\big)\ln\big(1+\tfrac{1}{2}\bar{N}\big) - \bar{N}\ln\bar{N} - \big(1-\tfrac{1}{2}\bar{N}\big)\ln\big(1-\tfrac{1}{2}\bar{N}\big) \quad : \ g = \tfrac{1}{2}.$$

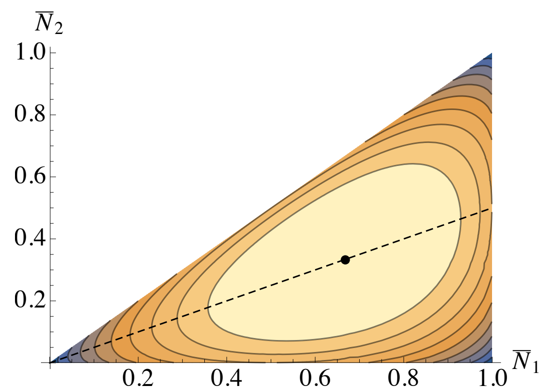
[4]Isakov 1994.

- The fermions produce the largest entropy when the system is half full. The entropy curve has a reflection symmetry at $\bar{N} = \frac{1}{2}$.
- The entropy of bosons is a monotonically increasing function $\bar{N}$. Its growth slows down to $\sim \ln \bar{N}$ for large $\bar{N}$.
- The maximum particle density for semions is twice that of fermions. Semions produce the largest entropy before the system is half full.

Example with two species of particles.

We first consider a system of hosts 1 and caps 2. The scaled configurational entropy reads

$$\bar{S}/k_\mathrm{B} = -\big(1-\bar{N}_1\big)\ln\big(1-\bar{N}_1\big) - \bar{N}_2 \ln \bar{N}_2 - \big(\bar{N}_1 - \bar{N}_2\big)\ln\big(\bar{N}_1 - \bar{N}_2\big).$$



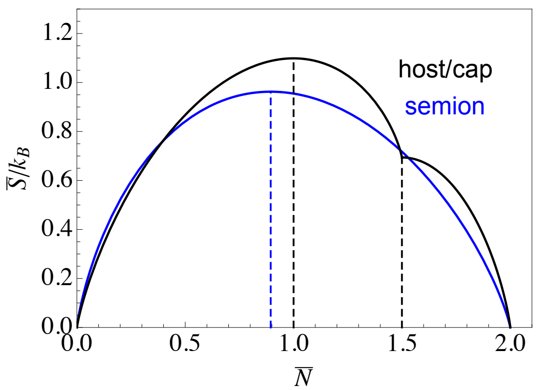
- The cap population cannot exceed the host population, which implies $0 \leq \bar{N}_2 \leq \bar{N}_1 \leq 1$.
- Contour lines are at $\bar{S}/k_\mathrm{B} = 0.1, \ldots, 0.9$
- The entropy maximum at given host density $\bar{N}_1$ is realized for cap density $\bar{N}_2 = \frac{1}{2}\bar{N}_1$.
- Global entropy maximum: $\bar{S}/k_\mathrm{B} = \ln 3$ for $\bar{N}_1 = \frac{2}{3}$, $\bar{N}_2 = \frac{1}{3}$.

Semions versus hosts and caps.

A system of N_A orbitals can accommodate a maximum of $2N_A$ spinons or $2N_A$ hosts and caps (N_A particles of each category).

It is correct to state that each orbital can accommodate one host and one cap, but incorrect to state that each orbital can accommodate two semions.

The graph compares the configurational entropy plotted versus average population density of semions and host/cap combinations.



– Semions produce the highest entropy $\bar{S}/k_{\rm B} \simeq 0.962$ at $\bar{N} \simeq 0.894$.

– For host/cap combinations we set $\bar{N} = \bar{N}_1 + \bar{N}_2$.

– Host/cap combinations at $0 < \bar{N} < 1.5$ produce the highest entropy when $\bar{N}_2 = \frac{1}{2}\bar{N}_1$.

– At higher population density, the host population is at its maximum, $\bar{N}_1 = 1$ and the cap population increases: $\frac{1}{2} < \bar{N}_2 < 1$.

– Hosts and caps produce the highest entropy $\bar{S}/k_{\rm B} = \ln 3 \simeq 1.098$ at $\bar{N} = 1$.

– At $\bar{N} = 1.5$, the largest host/cap entropy dips slightly below the semion entropy.

– At low population densities the semion entropy is slightly higher than the maximum host/cap entropy.