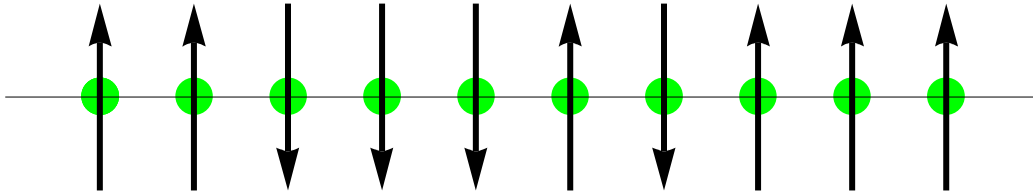


Spin 1/2 particles and Gaussian distribution
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We consider N spins with spin 1/2 in the presence of a magnetic field. There are two spin state with the up-state (the magnetic moment m) and the down-state (the energy $-m$) for each spin. We discuss the number of the spin arrangement for N spins.

1. Introduction

We use the following simple notation for a single state of the system of N sites.



Every distinct state of the system is contained in a symbolic product of N factors.

$$(\uparrow_1 + \downarrow_1)(\uparrow_2 + \downarrow_2)(\uparrow_3 + \downarrow_3) \cdots (\uparrow_N + \downarrow_N).$$

which is called a generating function. It generates the state of the system. The multiplication rule is defined by

$$(\uparrow_1 + \downarrow_1)(\uparrow_2 + \downarrow_2) = \uparrow_1 \uparrow_2 + \uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2 + \downarrow_1 \downarrow_2$$

((Note))

It is convenient to expand

$$(\uparrow_1 a + \downarrow_1 b)(\uparrow_2 a + \downarrow_2 b) = \uparrow_1 \uparrow_2 a^2 + (\uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2)ab + \downarrow_1 \downarrow_2 b^2$$

Instead of $(\uparrow_1 + \downarrow_1)(\uparrow_2 + \downarrow_2) = \uparrow_1 \uparrow_2 + \uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2 + \downarrow_1 \downarrow_2$.

The coefficient of a^2 is $\uparrow_1 \uparrow_2$

The coefficient of ab is $(\uparrow_1 \downarrow_2 + \downarrow_1 \uparrow_2)$

The coefficient of b^2 is $\downarrow_1 \downarrow_2$

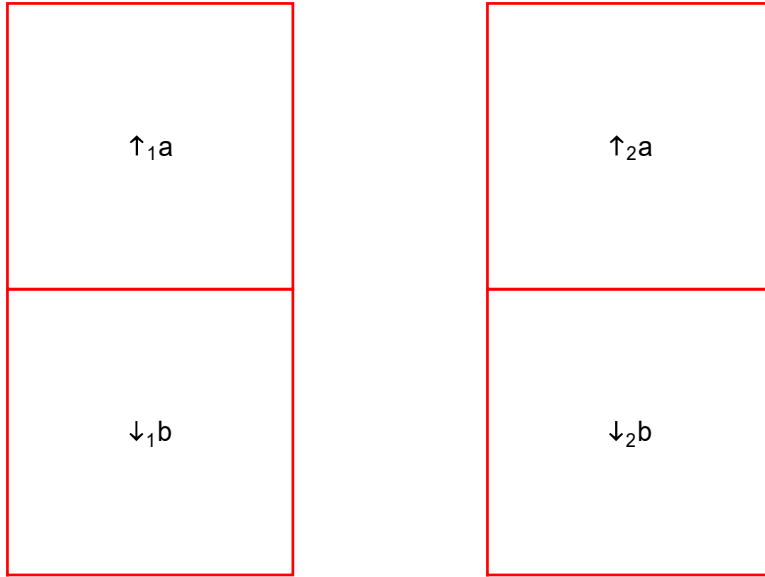


Fig. There are two possibilities: spin up state and spin down state.

We use the following notation

$$N_{\uparrow} + N_{\downarrow} = N, \quad N_{\uparrow} - N_{\downarrow} = 2s$$

or

$$N_{\uparrow} = \frac{N}{2} + s, \quad N_{\downarrow} = \frac{N}{2} - s$$

$$N = 3$$

$$-3 \leq 2s \leq 3, \quad s = \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2},$$

For a system of two elementary magnets, we obtain the four possible states,

$$\uparrow_1 \uparrow_2 \quad (1) \quad M = 2m \quad 2s = 2$$

$$\uparrow_1 \downarrow_2, \downarrow_1 \uparrow_2 \quad (2) \quad M = 0 \quad 2s = 0$$

$$\downarrow_1 \downarrow_2 \quad (1) \quad M = -2m \quad 2s = -2$$

The sum is not a state but is a way of listing the four possible states of the system

The generating function for the states of a system of three magnets.

$$(\uparrow_1 + \downarrow_1)(\uparrow_2 + \downarrow_2)(\uparrow_3 + \downarrow_3)$$

or

$$\uparrow_1 \uparrow_2 \uparrow_3 \quad (1) \qquad M = 3m \qquad 2s = 3$$

$$\uparrow_1 \uparrow_2 \downarrow_3, \quad \uparrow_1 \downarrow_2 \uparrow_3, \quad \downarrow_1 \uparrow_2 \uparrow_3 \quad (3) \qquad M = m \qquad 2s = 1$$

$$\uparrow_1 \downarrow_2 \downarrow_3, \quad \downarrow_1 \uparrow_2 \downarrow_3, \quad \downarrow_1 \downarrow_2 \uparrow_3 \quad (3) \qquad M = -m \qquad 2s = -1$$

$$\downarrow_1 \downarrow_2 \downarrow_3 \quad (1) \qquad M = -3m \qquad 2s = -3$$

There are $2^3 = 1 + 3 + 3 + 1 = 8$ states.

$N = 4$

$$-4 \leq 2s \leq 4, \quad s = 2, 1, 0, -1, -2$$

There are $2^4 = 16$ states.

$$(\uparrow_1 + \downarrow_1)(\uparrow_2 + \downarrow_2)(\uparrow_3 + \downarrow_3)(\uparrow_4 + \downarrow_4)$$

$$\uparrow_1 \uparrow_2 \uparrow_3 \uparrow_4 \quad (1) \qquad M = 4m \qquad 2s = 4$$

$$\uparrow_1 \uparrow_2 \uparrow_3 \downarrow_4, \quad \uparrow_1 \uparrow_2 \downarrow_3 \uparrow_4, \quad \uparrow_1 \downarrow_2 \uparrow_3 \uparrow_4, \quad \downarrow_1 \uparrow_2 \uparrow_3 \uparrow_4 \quad (4) \qquad M = 2m \qquad 2s = 2$$

$$\uparrow_1 \uparrow_2 \downarrow_3 \downarrow_4, \quad \uparrow_1 \downarrow_2 \uparrow_3 \downarrow_4, \quad \uparrow_1 \downarrow_2 \downarrow_3 \uparrow_4, \quad \downarrow_1 \downarrow_2 \uparrow_3 \uparrow_4 \qquad M = 0m \qquad 2s = 0$$

$$\downarrow_1 \uparrow_2 \downarrow_3 \uparrow_4, \quad \downarrow_1 \uparrow_2 \uparrow_3 \downarrow_4 \quad (6)$$

$$\downarrow_1 \downarrow_2 \downarrow_3 \uparrow_4, \quad \downarrow_1 \downarrow_2 \uparrow_3 \downarrow_4, \quad \downarrow_1 \uparrow_2 \downarrow_3 \downarrow_4, \quad \uparrow_1 \downarrow_2 \downarrow_3 \downarrow_4 \quad (4) \qquad M = -2m \qquad s = -2$$

$$\downarrow_1 \downarrow_2 \downarrow_3 \downarrow_4 (1)$$

$$M = -4m \quad 2s = -4$$

Note that

$$2^4 = 1 + 4 + 6 + 4 + 1 = 16$$

In the presence of magnetic field B , the up-state has an energy $-mB$, while the down-state has an energy mB . The total energy E is

$$\begin{aligned} E &= -mBN_{\uparrow} + mBN_{\downarrow} \\ &= -mB(N_{\uparrow} - N_{\downarrow}) \\ &= -2mBs \\ &= -MB \end{aligned}$$

where

$$M = 2sm$$

with

$$-\frac{N}{2} \leq s \leq \frac{N}{2}$$

2. Enumeration of states and the multiplicity function

We use the word “spin” as a shorthand for elementary magnet. We assume that N is an even number. We need a mathematical expansion for the number of states with

$$N_{\uparrow} = \frac{N}{2} + s, \quad N_{\downarrow} = \frac{N}{2} - s$$

where s is an integer.

$$N_{\uparrow} - N_{\downarrow} = 2s$$

which is called the “spin excess.”

The total magnetization M is given by

$$\begin{aligned}
M &= mN_{\uparrow} + (-m)N_{\downarrow} \\
&= m(N_{\uparrow} - N_{\downarrow}) \\
&= 2ms
\end{aligned}$$

where

$$s = -\frac{N}{2}, -\frac{N}{2} + 1, -\frac{N}{2} + 2, \dots, \frac{N}{2} - 1, \frac{N}{2},$$

We may drop the site labels when we are interested in how many of the magnets in a state are up or down, and not in which particular sites have magnets up or down.

$$(\uparrow + \downarrow)^N = (x + y)^N$$

where $x = \uparrow$ and $y = \downarrow$.

$$\begin{aligned}
(x + y)^N &= \sum_{s=-N/2}^{N/2} \frac{N!}{(N_{\uparrow})! (N_{\downarrow})!} x^{N_{\uparrow}} y^{N_{\downarrow}} \\
&= \sum_{s=-N/2}^{N/2} \frac{N!}{(\frac{1}{2}N + s)! (\frac{1}{2}N - s)!} x^{\frac{1}{2}N + s} y^{\frac{1}{2}N - s} \\
&= \sum_{s=-N/2}^{N/2} \frac{N!}{(\frac{1}{2}N + s)! (\frac{1}{2}N - s)!} x^{\frac{1}{2}N + s} y^{\frac{1}{2}N - s}
\end{aligned}$$

where

$$N_{\uparrow} = \frac{N}{2} + s, \quad N_{\downarrow} = \frac{N}{2} - s$$

Note that

$${}_n C_r = \frac{n!}{(n-r)! r!} = \frac{N!}{N_{\uparrow}! N_{\downarrow}!}$$

where

$$n = N, \quad N_{\uparrow} = N - r = \frac{N}{2} + s, \quad N_{\downarrow} = r = \frac{N}{2} - s$$

$$N_{\uparrow} - N_{\downarrow} = N - 2r = 2s$$

The coefficient of the term in $\uparrow^{\frac{1}{2}N+s} \downarrow^{\frac{1}{2}N-s}$ is the number of states having

$$N_{\uparrow} = N - r = \frac{N}{2} + s, \quad (\text{magnets up})$$

$$N_{\downarrow} = r = \frac{N}{2} - s. \quad (\text{magnets down})$$

This class of states has spin excess $N_{\uparrow} - N_{\downarrow} = 2s$ and net magnetic moment $2sm$. We denote the number of states in this class by $g(N, s)$

$$g(N, s) = \frac{N!}{(\frac{1}{2}N + s)!(\frac{1}{2}N - s)!} = \frac{N!}{(N_{\uparrow})!(N_{\downarrow})!}$$

We call $g(N, s)$ the multiplicity function. When a magnetic field is applied to the spin systems, state of different values of S have different values of the energy, so that our g is equal to the multiplicity of an energy level in a magnetic field.

Since

$$(x + y)^N = \sum_{s=-N/2}^{N/2} g(N, s) x^{\frac{1}{2}N+s} y^{\frac{1}{2}N-s}$$

we have the total number states for $x = y = 1$

$$2^N = \sum_{s=-N/2}^{N/2} g(N, s)$$

3. Stirling's formula (I)

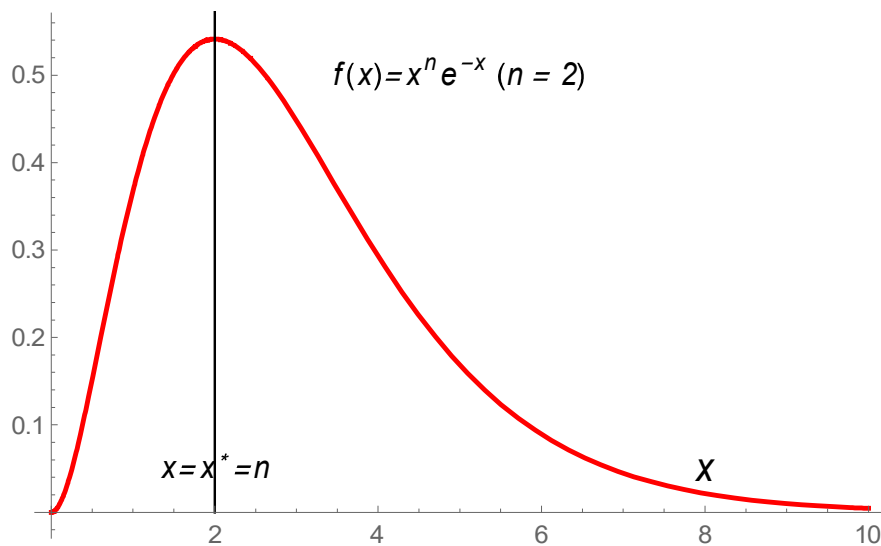
The integral formula provides one such convenient expression, namely

$$n! = \int_0^{\infty} x^n e^{-x} dx$$

Note the Laplace transformation,

$$\int_0^{\infty} t^n e^{-st} dt = \frac{n!}{s^{n+1}}$$

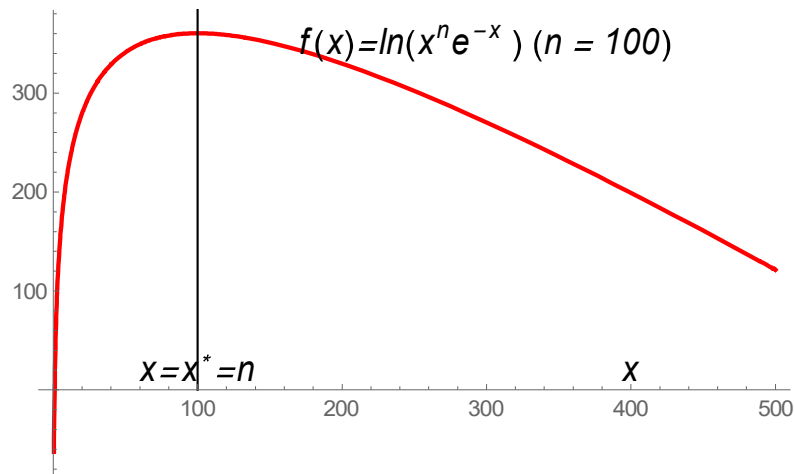
Consider the integrand $F = x^n e^{-x}$, when n is large. Then x^n is a rapidly increasing function of x , while e^{-x} is a rapidly decreasing function of x . Hence F is a function which exhibits a sharp maximum for some value $x = x^* = n$, and falls off rapidly for x appreciably removed from $x = x^*$.



$$F(x) = x^n e^{-x},$$

$$F'(x) = -x^{n-1} e^{-x} (x - n)$$

It is equivalent and more convenient to work with $\ln F$. Since $\ln F$ is a monotonically increasing function of F , a maximum in $\ln F$ corresponds to a maximum of F .



To find this maximum, put

$$\frac{d \ln F}{dx} \Big|_{x=x^*} = 0 \quad \text{or} \quad \frac{d \ln F(x^*)}{dx^*} = 0$$

or

$$\frac{d}{dx^*} (n \ln x^* - x^*) = \frac{n}{x^*} - 1 = 0$$

Hence $x^* = n$.

The second derivative is negative at $x = x^*$.

$$\begin{aligned} \frac{d^2 \ln F(x^*)}{dx^{*2}} &= \frac{d}{dx^*} \frac{F'(x^*)}{F(x^*)} \\ &= \frac{F''(x^*)F(x^*) - [F'(x^*)]^2}{[F(x^*)]^2} \\ &= \frac{F''(x^*)}{F(x^*)} \\ &= -\frac{n}{x^{*2}} \\ &= -\frac{1}{n} \\ &= -\frac{1}{\sigma_{x^*}^2} \end{aligned}$$

or

$$\sigma_{x^*} = \sqrt{n}$$

Then the function $\ln F$ can be described in the neighborhood of $x = x^*$,

$$\begin{aligned}\ln F(x) &= \ln F(x^*) + (x - x^*) \frac{d \ln F(x^*)}{dx^*} + \frac{1}{2!} (x - x^*)^2 \frac{d^2 \ln F(x^*)}{dx^{*2}} \\ &= \ln F(x^*) - \frac{1}{2\sigma_{x^*}^2} (x - x^*)^2\end{aligned}$$

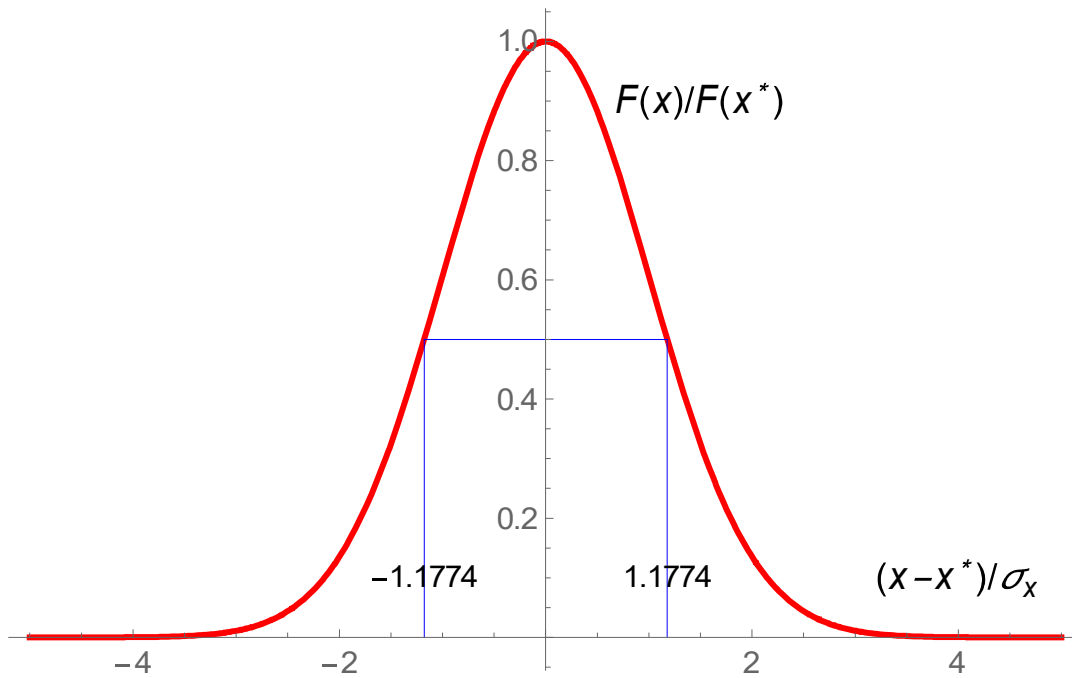
or

$$F(x) = F(x^*) \exp\left[-\frac{1}{2\sigma_{x^*}^2} (x - x^*)^2\right]$$

Gaussian distribution centered at $x = x^* = n$ with the width $2\sqrt{2\ln 2}\sigma_x = 2.3548\sigma_x$

$$\ln 2 = \frac{1}{2\sigma_x^2} (x - x^*)^2]$$

$$\frac{x - x^*}{\sigma_x} = \pm\sqrt{2\ln 2} = \pm\sqrt{2\ln 2} = \pm 1.17741.$$



Then the integral becomes

$$\begin{aligned}
 n! &= \int_0^{\infty} F(x) dx \\
 &\approx \int_0^{\infty} F(x^*) \exp\left[-\frac{1}{2\sigma_{x^*}^2} (x - x^*)^2\right] dx \\
 &= F(x^*) \int_0^{\infty} \exp\left[-\frac{1}{2\sigma_{x^*}^2} (x - x^*)^2\right] dx \\
 &= \sqrt{2\pi} \sigma_{x^*} F(x^*) \\
 &= \sqrt{2\pi n} F(x^*) \\
 &= \sqrt{2\pi n} n^n e^{-n}
 \end{aligned}$$

for $n \gg 1$.

The Stirling's formula

$$n! = \sqrt{2\pi n} \left(\frac{n}{e}\right)^n$$

It can be also be written in the form

$$\begin{aligned}
 \ln n! &= n(\ln n - 1) + \frac{1}{2} \ln(2\pi n) \\
 &= (n + \frac{1}{2}) \ln n - n + \frac{1}{2} \ln(2\pi) \\
 &\approx n(\ln n - 1)
 \end{aligned}$$

((Example))

n	Log[n !]	$(n + \frac{1}{2}) \text{Log}[n] - n + \frac{1}{2} \text{Log}[2 \pi]$
10	15.1044	15.0961
20	42.3356	42.3315
30	74.6582	74.6555
40	110.321	110.319
50	148.478	148.476
60	188.628	188.627
70	230.439	230.438
80	273.673	273.672
90	318.153	318.152
100	363.739	363.739

n	Log[n !]	$(n + \frac{1}{2}) \text{Log}[n] - n + \frac{1}{2} \text{Log}[2 \pi]$
100	363.739	363.739
200	863.232	863.232
300	1414.91	1414.91
400	2000.5	2000.5
500	2611.33	2611.33
600	3242.28	3242.28
700	3889.95	3889.95
800	4551.95	4551.95
900	5226.48	5226.48
1000	5912.13	5912.13

n	$\text{Log}[n!]$	$(n + \frac{1}{2}) \text{Log}[n] - n + \frac{1}{2} \text{Log}[2\pi]$
1000	5912.13	5912.13
2000	13 206.5	13 206.5
3000	21 024.	21 024.
4000	29 181.3	29 181.3
5000	37 591.1	37 591.1
6000	46 202.4	46 202.4
7000	54 981.	54 981.
8000	63 903.	63 903.
9000	72 950.3	72 950.3
10 000	82 108.9	82 108.9

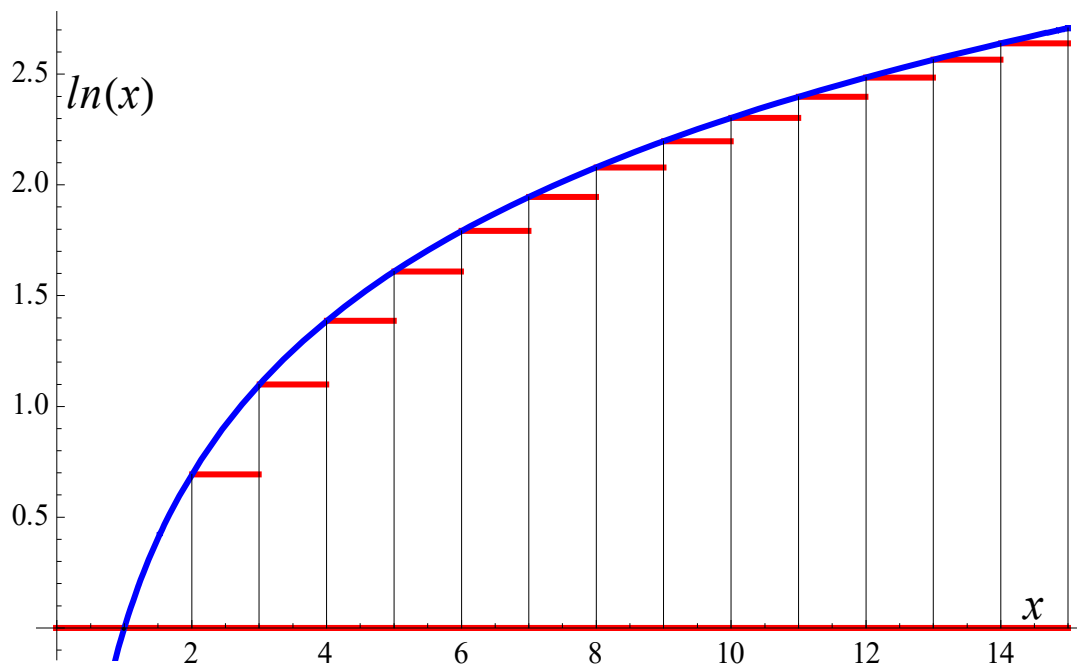
4. Stirling's formula (II)

H.J.W. Muller-Kristen, Basic of Statistical Physics (World Scientific, 2010).

We start with

$$\ln(n!) = \ln[1 \times 2 \times 3 \times \dots \times n] = \sum_{i=1}^N \ln(i)$$

which is equal to the area under the staircase in this Fig.



Thus, to a good approximation:

$$\ln(n!) = \int_1^n \ln x dx = [x \ln x - x]_1^n = n(\ln n - 1)$$

where n is large.

5. Sharpness of the multiplicity function

We show that for a very large system, the function $g(N, s)$ is peaked very sharply about $s = 0$. using the Stirling's formula,

$$\begin{aligned} \ln[g(N, s)] &= \ln \frac{N!}{N_+! N_-!} \\ &= \ln(N!) - \ln(N_+!) - \ln(N_-!) \\ &= (N + \frac{1}{2}) \ln N - N + \frac{1}{2} \ln(2\pi) \\ &\quad - (N_\uparrow + \frac{1}{2}) \ln N_\uparrow + N_\uparrow - \frac{1}{2} \ln(2\pi) \\ &\quad - (N_\downarrow + \frac{1}{2}) \ln N_\downarrow + N_\downarrow - \frac{1}{2} \ln(2\pi) \\ &= (N + \frac{1}{2}) \ln N - (N_\uparrow + \frac{1}{2}) \ln N_\uparrow - (N_\downarrow + \frac{1}{2}) \ln N_\downarrow - \frac{1}{2} \ln(2\pi) \\ &= (N_\uparrow + N_\downarrow + \frac{1}{2}) \ln N - (N_\uparrow + \frac{1}{2}) \ln N_\uparrow - (N_\downarrow + \frac{1}{2}) \ln N_\downarrow - \frac{1}{2} \ln(2\pi) \\ &= \{(N_\uparrow + \frac{1}{2}) + (N_\downarrow + \frac{1}{2}) - \frac{1}{2}\} \ln N - (N_\uparrow + \frac{1}{2}) \ln N_\uparrow - (N_\downarrow + \frac{1}{2}) \ln N_\downarrow - \frac{1}{2} \ln(2\pi) \\ &= \frac{1}{2} \ln\left(\frac{1}{2\pi N}\right) - (N_\uparrow + \frac{1}{2}) \ln \frac{N_\uparrow}{N} - (N_\downarrow + \frac{1}{2}) \ln \frac{N_\downarrow}{N} \end{aligned}$$

We use the formula

$$\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} + \dots$$

for $|x| \ll 1$. Using this, we get

$$\begin{aligned}
\ln \frac{N_{\uparrow}}{N} &= \ln \left(\frac{\frac{1}{2}N + s}{N} \right) \\
&= \ln \left[\frac{1}{2} \left(1 + \frac{2s}{N} \right) \right] \\
&= -\ln 2 + \ln \left(1 + \frac{2s}{N} \right) \\
&= -\ln 2 + \frac{2s}{N} - \frac{1}{2} \left(\frac{2s}{N} \right)^2
\end{aligned}$$

Similarly,

$$\begin{aligned}
\ln \frac{N_{\downarrow}}{N} &= \ln \left(\frac{\frac{1}{2}N - s}{N} \right) \\
&= \ln \left[\frac{1}{2} \left(1 - \frac{2s}{N} \right) \right] \\
&= -\ln 2 + \ln \left(1 - \frac{2s}{N} \right) \\
&= -\ln 2 - \frac{2s}{N} - \frac{1}{2} \left(\frac{2s}{N} \right)^2
\end{aligned}$$

On substitution, we obtain

$$\begin{aligned}
\ln[g(N, s)] &= \frac{1}{2} \ln \left(\frac{1}{2\pi N} \right) - (N_{\uparrow} + \frac{1}{2}) \ln \frac{N_{\uparrow}}{N} - (N_{\downarrow} + \frac{1}{2}) \ln \frac{N_{\downarrow}}{N} \\
&= \frac{1}{2} \ln \left(\frac{1}{2\pi N} \right) - (N_{\uparrow} + \frac{1}{2}) \left[-\ln 2 + \frac{2s}{N} - \frac{1}{2} \left(\frac{2s}{N} \right)^2 \right] - (N_{\downarrow} + \frac{1}{2}) \left[-\ln 2 - \frac{2s}{N} - \frac{1}{2} \left(\frac{2s}{N} \right)^2 \right] \\
&= \frac{1}{2} \ln \left(\frac{1}{2\pi N} \right) + (N_{\uparrow} + N_{\downarrow} + 1) \ln 2 - \frac{2s}{N} (N_{\uparrow} + \frac{1}{2} - N_{\downarrow} - \frac{1}{2}) + \frac{1}{2} \left(\frac{2s}{N} \right)^2 (N_{\uparrow} + \frac{1}{2} + N_{\downarrow} + \frac{1}{2}) \\
&= \frac{1}{2} \ln \left(\frac{1}{2\pi N} \right) + (N + 1) \ln 2 - \frac{4s^2}{N} + \frac{2s^2}{N^2} (N + 1) \\
&\approx \frac{1}{2} \ln \left(\frac{1}{2\pi N} \right) + N \ln 2 - \frac{2s^2}{N} + \frac{1}{2} \ln 2^2 \\
&= \frac{1}{2} \ln \left(\frac{2^2}{2\pi N} \right) + N \ln 2 - \frac{2s^2}{N}
\end{aligned}$$

Hence,

$$\ln[g(N,s)] = \ln[2^N (\frac{2}{\pi N})^{1/2}] - \frac{2s^2}{N}$$

We write this result as

$$g(N,s) = 2^N (\frac{2}{\pi N})^{1/2} \exp(-\frac{2s^2}{N})$$

Such a distribution of values of s is called a Gaussian distribution. The exact values of $g(N,s=0)$ is given by

$$g(N,0) = \frac{N!}{\left(\frac{N}{2}\right)! \left(\frac{N}{2}\right)!}$$

We consider the Gaussian distribution $f(s,\sigma)$ defined by

$$\sum_s g(N,s) = 2^N \approx \int_{-\infty}^{\infty} g(N,s) ds = 2^N \int_{-\infty}^{\infty} f(s,\sigma) ds$$

where

$$f(s,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp[-\frac{s^2}{2\sigma^2}] \quad \text{(Gaussian distribution function)}$$

with

$$\sigma = \frac{\sqrt{N}}{2}.$$

Note that

$$\exp(-\frac{2s^2}{N}) = \exp(-\frac{s^2}{2\sigma^2}), \quad \sqrt{\frac{2}{\pi N}} = \frac{1}{\sqrt{2\pi}\sigma}$$

Then $g(N,s)$ can be written as

$$g(N, s) = 2^N \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{s^2}{2\sigma^2}\right) = 2^N f(s, \sigma)$$

The function $f(s, \sigma)$ is normalized as

$$\int_{-\infty}^{\infty} f(s, \sigma) ds = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{s^2}{2\sigma^2}\right] ds = 1$$

If all the states are equally probable, then the probability

$$P(N, s) = \frac{1}{2^N} g(N, s) = f(s, \sigma)$$

is a Gaussian distribution for large N system.

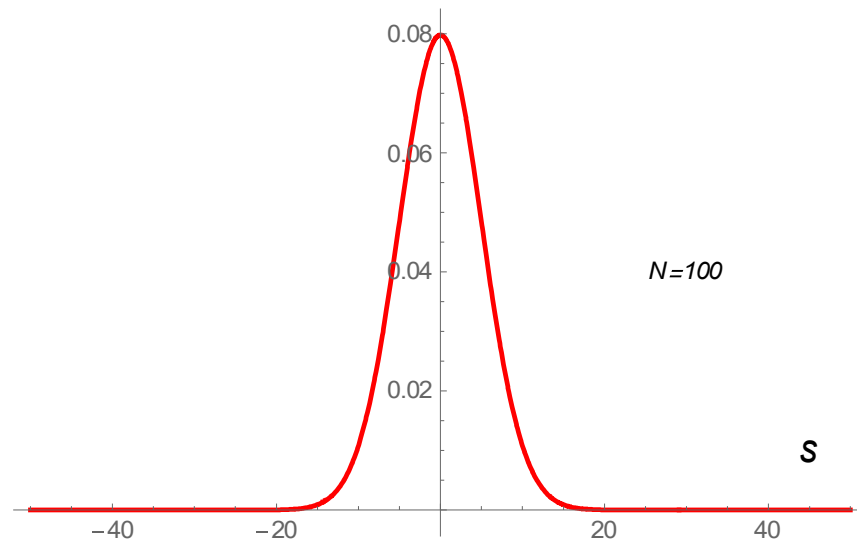


Fig. The probability $P(N, s)$ as a function of s . $N = 100$.

We consider the average

$$\langle s \rangle = 0$$

$$\begin{aligned}
\langle s^2 \rangle &= \sum_s s^2 P(N, s) \\
&= \int_{-\infty}^{\infty} s^2 f(s, \sigma) ds \\
&= \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} s^2 \exp\left[-\frac{s^2}{2\sigma^2}\right] ds \\
&= \sigma^2 \\
&= \frac{N}{4}
\end{aligned}$$

Hence, we have

$$\langle (2s)^2 \rangle = N$$

which is the mean square spin excess. The root mean square spin excess is

$$\langle (2s)^2 \rangle^{1/2} = \sqrt{N}$$

The fractional fluctuation:

$$F = \frac{\langle (2s)^2 \rangle^{1/2}}{N} = \frac{1}{\sqrt{N}}$$

The larger N is the smaller is the fractional fluctuation.