Thermal distributions 1

Tossing coins, microstates, and macrostates

Modern physics for engineers

David Miller

Tossing coins

- We toss a coin 4 times
  - There are 16 possibilities
    - shown using ↑ for heads
      - and ↓ for tails
- We call each possible set of 4 outcomes
  - a microstate

Microstate
↑↑↑↑
↑↑↑↓
↑↑↓↑
↑↓↑↑
↓↑↑↑
↑↑↓↓
↑↓↑↓
↓↑↑↓
↑↓↓↑
↓↑↓↑
↓↓↑↑
↓↓↓↑
↓↓↑↓
↓↑↓↓
↑↓↓↓
↓↓↓↓

Tossing coins

We can group these microstates into
  macrostates
   each containing all microstates corresponding to
    a particular number of heads and tails

Microstate	Macrostate
↑↑↑↑	4 up (“heads”)
↑↑↑↓ ↑↑↓↑ ↑↓↑↑ ↓↑↑↑	3 up (“heads”) 1 down (“tails”)
↑↑↓↓ ↑↓↑↓ ↓↑↑↓ ↑↓↓↑ ↓↑↓↑ ↓↓↑↑	2 up (“heads”) 2 down (“tails”)
↓↓↓↑ ↓↓↑↓ ↓↑↓↓ ↑↓↓↓	1 up (“heads”) 3 down (“tails”)
↓↓↓↓	4 down (“tails”)

Tossing coins

The number of microstates
in each macrostate
is called the
multiplicity
of the macrostate

Microstate	Macrostate	Multiplicity
↑↑↑↑	4 up ("heads")	1
↑↑↑↓ ↑↑↓↑ ↑↓↑↑ ↓↑↑↑	3 up ("heads") 1 down ("tails")	4
↑↑↓↓ ↑↓↑↓ ↓↑↑↓ ↑↓↓↑ ↓↑↓↑ ↓↓↑↑	2 up ("heads") 2 down ("tails")	6
↓↓↓↑ ↓↓↑↓ ↓↑↓↓ ↑↓↓↓	1 up ("heads") 3 down ("tails")	4
↓↓↓↓	4 down ("tails")	1

Tossing coins

For each macrostate

- we can also write an
  - excess
    - which is the "excess" number of heads compared to tails

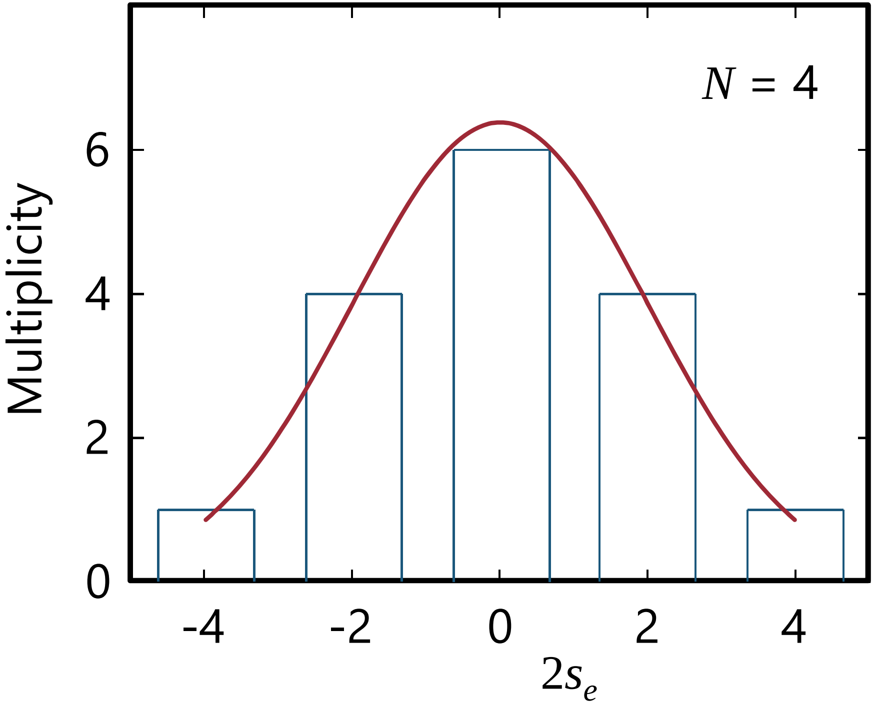
We can write the excess as $2s_e$

- where s_e is the difference in the number of heads
  - compared to the average

Microstate	Macrostate	Multiplicity	Excess, $2s_e$
↑↑↑↑	4 up ("heads")	1	4
↑↑↑↓ ↑↑↓↑ ↑↓↑↑ ↓↑↑↑	3 up ("heads") 1 down ("tails")	4	2
↑↑↓↓ ↑↓↑↓ ↓↑↑↓ ↑↓↓↑ ↓↑↓↑ ↓↓↑↑	2 up ("heads") 2 down ("tails")	6	0
↓↓↓↑ ↓↓↑↓ ↓↑↓↓ ↑↓↓↓	1 up ("heads") 3 down ("tails")	4	-2
↓↓↓↓	4 down ("tails")	1	-4

Tossing coins

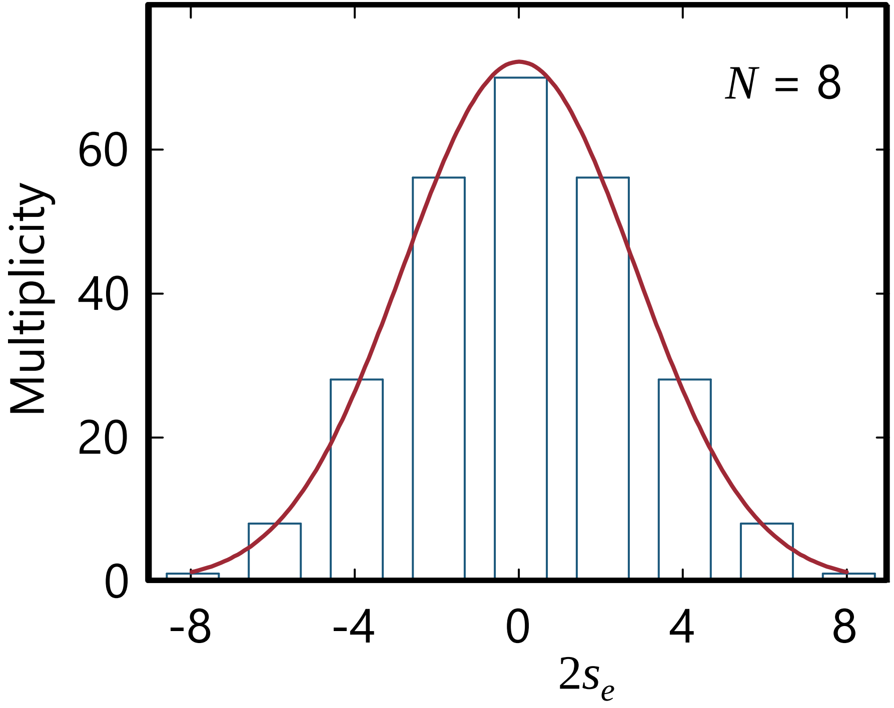
We can plot the multiplicity
- here for $N = 4$ coin tosses
  - as a function of the "excess"
    - also showing a curve of a Gaussian approximation



Tossing coins

Increasing N gives

- much larger peak multiplicity
  - and
- a wider curve
  - though narrower relative to N



Tossing coins

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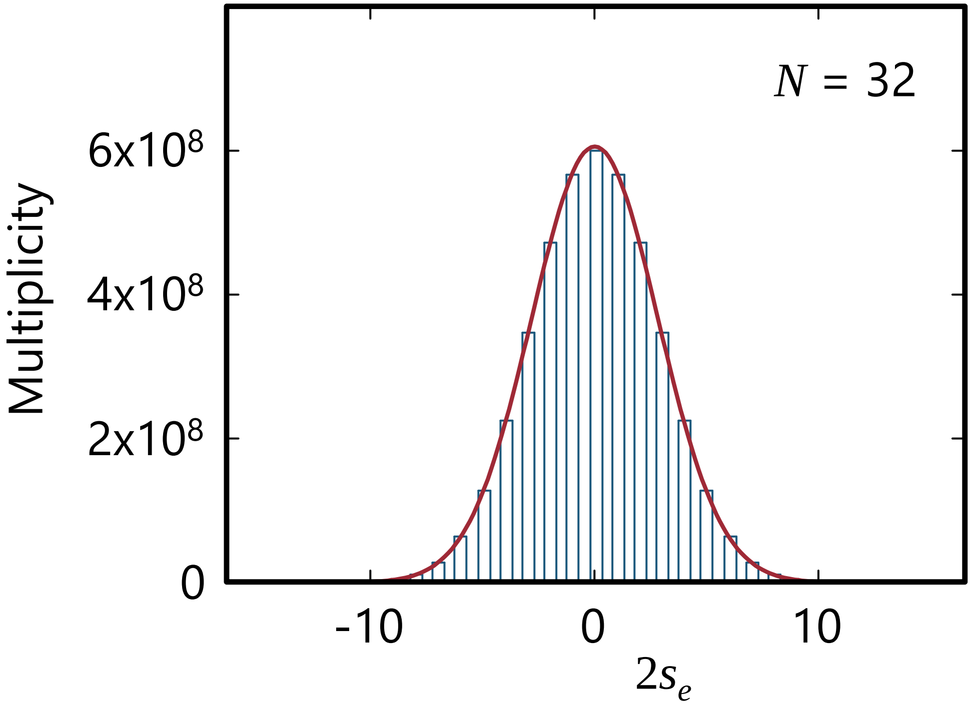

Tossing coins

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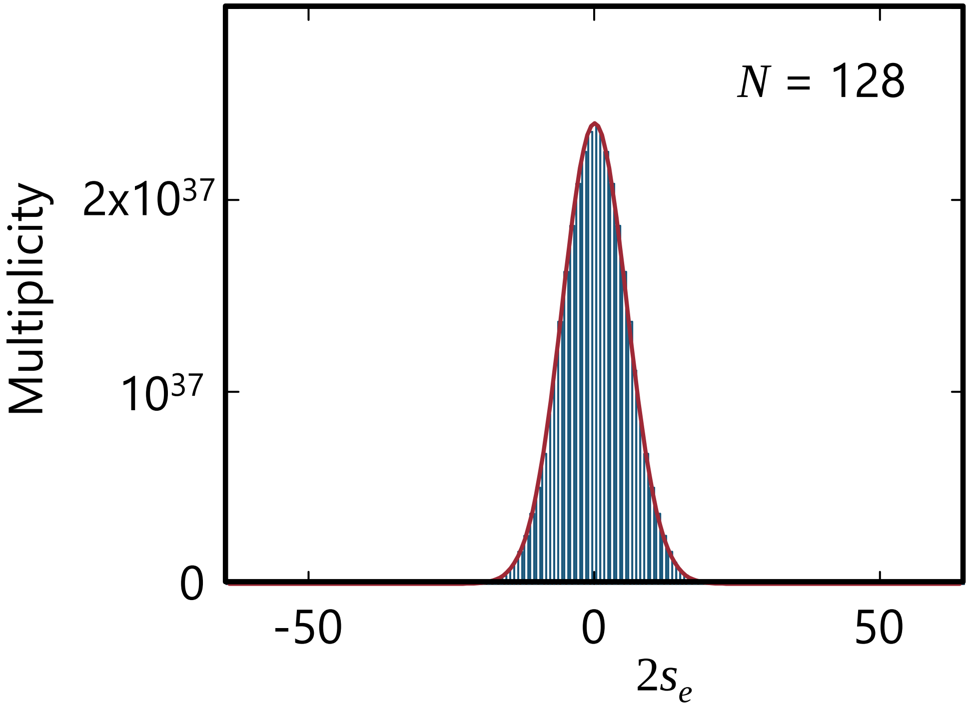
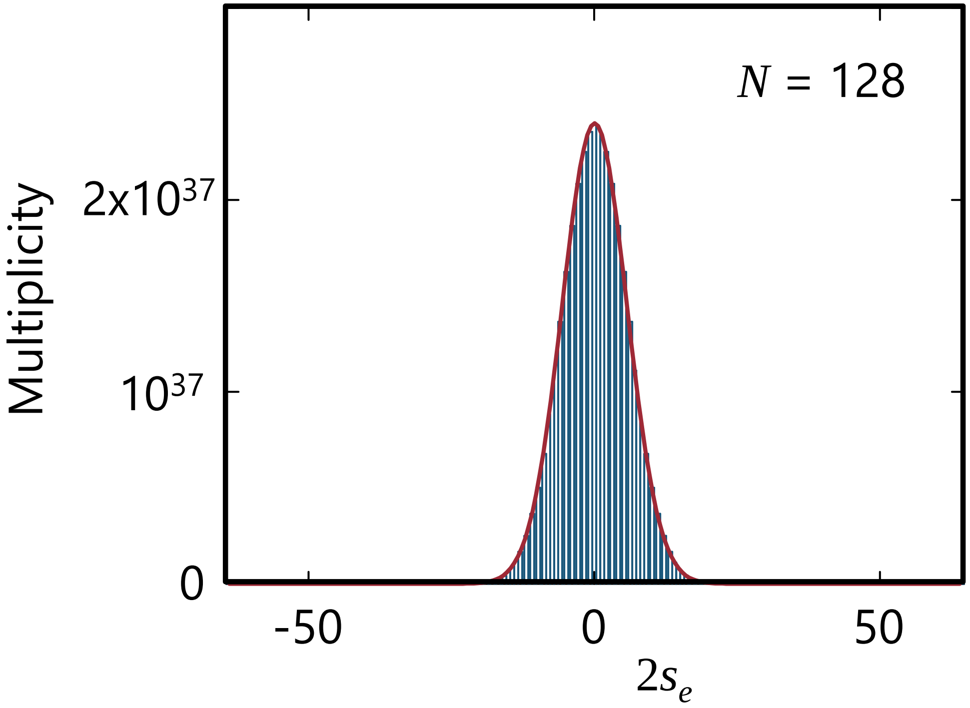


Tossing coins

- The multiplicity drops as
  - the magnitude of the difference between heads and tails increases
- The most likely outcome is equal heads and tails
  - Outcomes with approximately equal heads and tails
    - dominate as N increases



Thermal distributions 1

Binomial distribution and Stirling's approximation

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Binomial distribution

Binomial distribution

When tossing coins

- the formula for the number of microstates in a macrostate
  - that is, the multiplicity of the macrostate
- is an example of the binomial distribution

Binomial distribution

Suppose we have N coins in a row

e.g., starting all "heads"

Take k of them, and flip them over

e.g., to "tails"

thereby creating two sets of coins in the row

"heads" and "tails"

Binomial distribution

There are

N ways we can choose the first coin to flip over

$N-1$ ways we can choose the second

and so, down to

$N-k+1$ for our kth choice

Multiplying these together gives us

$$N(N-1)(N-2)\ldots(N-k+1)=\frac{N!}{(N-k)!}$$

Binomial distribution

There are also $k!$ different orderings in which

we could have chosen which coins to flip over

while still leaving us the same sets of "heads" and "tails" in the row

so we divide by $k!$ giving

$$g = \frac{N!}{(N-k)!k!}$$

for the total number of different-looking rows of coins in which k of them are flipped over

which is the binomial distribution

Multiplicity of macrostates

This binomial distribution $g = \frac{N!}{(N-k)!k!}$

gives the multiplicity of a macrostate

corresponding to k "heads" and $N-k$ "tails"

We prefer to write this in terms of s_e, giving

$(N/2)+s_e$ for the number of "heads" and

$(N/2)-s_e$ for the number of "tails"

which gives $g(N,s_e) = \frac{N!}{\left(\frac{N}{2}+s_e\right)!\left(\frac{N}{2}-s_e\right)!}$

Multiplicity of macrostates

For example, for $k = 1$ "heads"

out of $N = 4$ coin tossings

$$g = \frac{N!}{(N-k)!k!} = \frac{4\times3\times2\times1}{(3\times2\times1)\times1} = 4$$

For $s_e = 2$, an "excess" $2s_e = 4$

which corresponds to 4 more "heads" than "tails"

$$g(N,s_e) = \frac{N!}{\left(\frac{N}{2}+s_e\right)!\left(\frac{N}{2}-s_e\right)!} = g(4,2) = \frac{4!}{(2+2)!0!} = \frac{4!}{4!0!} = 1$$

remembering $0! = 1$

Stirling's approximation

Stirling's approximation

For large N, we can use an approximation to this binomial distribution

which in turn is based on Stirling's approximation

For large N

$$\log(n!) \simeq \frac{1}{2}\log 2\pi n + n\log n - n$$

or equivalently

$$n! \simeq \sqrt{2\pi n}\,(n/e)^n$$

Approximate binomial distribution for large N

Using Stirling's approximation

together with the power series expansion

$$\log(1+x) \simeq x - x^2/2$$

after some algebra we can rewrite

$$g(N,s_e) = \frac{N!}{\left(\frac{N}{2}+s_e\right)!\left(\frac{N}{2}-s_e\right)!}$$

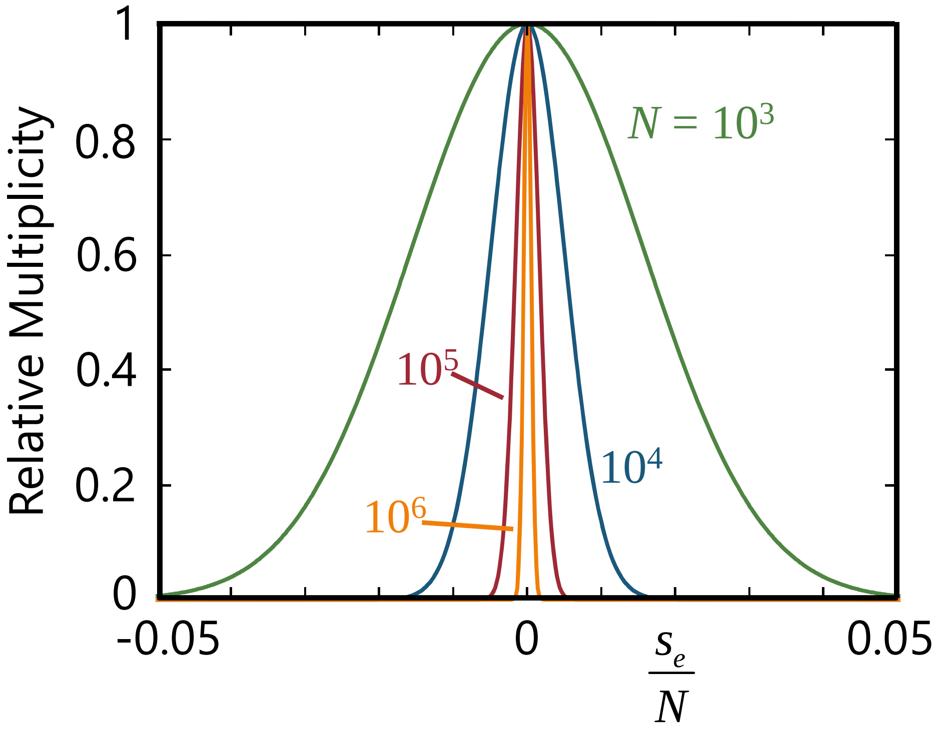
as

$$g(N,s_e) \simeq g(N,0)\exp\left(-\frac{2s_e^2}{N}\right)$$ with $$g(N,0) \simeq \sqrt{\frac{2}{\pi N}}\,2^N$$

Gaussian approximation

Using this Gaussian approximation

- as N becomes large
  - the absolute width does continue to grow
  - but the relative width becomes smaller



Width of the multiplicity distribution

From $g(N,s_e) \simeq g(N,0)\exp\left(-\frac{2s_e^2}{N}\right)$

we see the value of s_e for which

the distribution falls to $1/e^2$ of its peak value is

$$s_{ec} = \sqrt{N}$$

So, though the width of the distribution grows as $\sqrt{N}$

for the relative width we have $\frac{s_{ec}}{N} = \frac{1}{\sqrt{N}}$

Width of the multiplicity distribution

So, for example

- if we tossed a coin 10^{20} times
  - the average number of heads or tails would be
    - 0.5 within roughly 1 part in 10^{10}

Width of the multiplicity distribution

Note that

in terms of s_e / N

nearly all the microstates are found

in or very close

to the most likely macrostate

This is quite general behavior for such statistical systems

with large numbers of elements like this

Thermal distributions 1

Two-state spin systems and microstates

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Two-state spin systems and accessible microstates

Two-state spin systems

So far, we presumed that
- every such outcome of heads and tails
  - is possible
    - as indeed it is for tossing a coin

A related physical system would be
- a set of spins
  - such as a set of electrons
    - with negligible interaction between them

Two-state spin systems

- Just as each coin could be heads or tails
  - so each spin (or electron) could be
    - “spin-up” (“↑”) or
    - “spin-down” (“↓”)
- If there are no other constraints on spins being up or down
  - then we obtain the same kind of counting
    - for spins as for coins

Two-state spin systems and accessible microstates

Accessible states

- In real physical systems
  - different possible microstates
    - may have different energies
- If there is a fixed energy available
  - or there is some other constraint on energy
    - it may be that
      - not all the microstates we could write down
        - would be possible
          - or “accessible”

Accessible microstates

Given whatever physical constraints there are on the system

an accessible microstate is one that is physically possible

Accessible microstates

Now we make an important physical postulate

- which underlies our statistical analysis of physical systems
  - that are in equilibrium

By "equilibrium"

- we mean after everything has settled down
  - at least as we observe it macroscopically

Accessible microstates

For a physical system in equilibrium

each accessible microstate is equally probable

Two-state spin systems and energy

Non-equilibrium starting states

- We can start the system in a specific microstate
  - so its probability dominates over all the others
    - at that starting "non-equilibrium" condition

Non-equilibrium starting states

But once we have left the system to equilibrate

- on measuring the system
  - any accessible microstate is presumed to be
    - just as likely as any other

Two-state spin systems

We use the two-state spin system

as a model to understand the behavior of physical systems

presuming we can generalize to similar behaviors of

more complicated systems

without further formal proofs

Two-state spin systems

The key attribute we need

is to allow the microstates

to have energies that may not all be the same

Spins in a magnetic field

For our spin system

we imagine that we apply a magnetic field

of magnitude B

along the "up-down" axis of the spins

For a small magnet or spin

of magnetic moment (magnet "strength") μ_s

the energy of a "spin-up" "magnet" is

$$E_\mu = -\mu_s B$$

A spin with "spin-down"

will have exactly the opposite energy

Spins in a magnetic field

With some spins “up” and others “down”

the energy of equal numbers of “up” and “down” spins

will cancel out in the total energy, U

Hence, the total energy only depends on

the “spin excess” $2s_e$

specifically being

$$U\left(s_e\right) = -2\mu_s B s_e$$

We are interested in a closed physical system

in which this total energy U is fixed