AVERAGE VALUE

Let's go from multiplicity to probability

For our spin system,

$$\sum_s g(N,s) = 2^N$$

So probabilities summing to unity ($\underline{\underline{1}}$) are defined by $P(N,s) = 2^{-N} g(N,s)$

so that $\sum_s P(N,s) = 1$ for a given N

Def^n: AVERAGE value of a function $f(s)$ is

$$\boxed{\underbrace{\langle f \rangle}_{\text{new notation}} \equiv \sum_s P(N,s) f(s)}$$

For our system of spins, what's $\langle s \rangle$?

– Zero, by symmetry: $-s$ is just as likely as $+s$ (with zero magnetic field)

– What about $\langle s^2 \rangle$?

First, recall that $g(s,N) \underset{N\gg 1}{\approx} \sqrt{\frac{2}{\pi N}}\, 2^N \exp\left(-\frac{2s^2}{N}\right)$

i.e. our friend the "peaky" Gaussian approx. to discrete distribution jan14 2

Let's use our continuous approximation

$$\langle s^2\rangle = \int ds \left\{2^{-N} g(N,s)\right\} s^2$$

$$= \int ds\, s^2 \left\{2^{-N} \sqrt{\frac{2}{\pi N}}\, 2^N\right\} \exp\left(-\frac{2s^2}{N}\right)$$

$$= \sqrt{\frac{2}{\pi N}} \int ds\; s^2 \exp\left(-\frac{2s^2}{N}\right)$$

Change variables to $x^2 = \frac{2s^2}{N}$ i.e. $x = \frac{s}{\sqrt{N/2}}$.

Then

$$\langle s^2\rangle = \sqrt{\frac{2}{\pi N}} \left(\frac{N}{2}\right)^{3/2} \underbrace{\int dx\, x^2 e^{-x^2}}$$

do, or look up. Value $= \sqrt{\pi}/2$

$$\Rightarrow \boxed{\langle s^2\rangle = \frac{N}{4}}$$

Root-Mean-Square value?

$$s_{rms} \equiv \sqrt{\langle s^2\rangle - \langle s\rangle^2} = \sqrt{\langle s^2\rangle} \text{ here}$$

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

$$\Rightarrow \boxed{\frac{s_{rms}}{N} = \frac{1}{\sqrt{2N}}}$$

← fractional rms fluctuation from the mean ($\langle s\rangle = 0$)

Note that this is precisely the same as the half-width of the Gaussian! (This is special behavior specific to Gaussians.)

fundamental assumption of thermal physics

"a closed system is equally likely to be in any of the quantum states accessible to it"

Closed : constant U, N, V, external parameters

Accessible states : those that the system could find itself in on the timescale of the experiment

(some forms of a substance interconvert too slowly)
⇒ inaccessible.

Continuous approximation to discrete system

⇒ fix energy in range U to $U + \delta U$
\# particles N $N + \delta N$

* Thermodynamics is about specifying the macrostate (the state of the system of a macroscopic # of particles) and using statistics to derive those gross properties from microphysics. (the many microstates of all the little particles)

Use probabilities ;

* Definition: An ensemble of systems is a group of systems, all constructed alike, each of which is in precisely one of the accessible quantum states

deep

Theorem: (Ergodic Thm)
the ensemble average is the thermal average

Terminology:

Fixed N and U	*microcanonical* ensemble
Fixed N	*canonical
Neither	grand canonical

Probability of being in state of energy U, particle # N is $\frac{1}{g(N,U)} = P(N,U)$.

For microcanonical ensemble, this doesn't vary.

* Average of some quantity X is

$$\boxed{\langle X \rangle = \sum_s P(s)\, X(s)} \qquad \sum_s P(s) = 1$$

↑ some general state label (not necessarily spin excess!)

or $\langle X \rangle \to \int ds\, P(s)\, X(s)$ in continuous approx

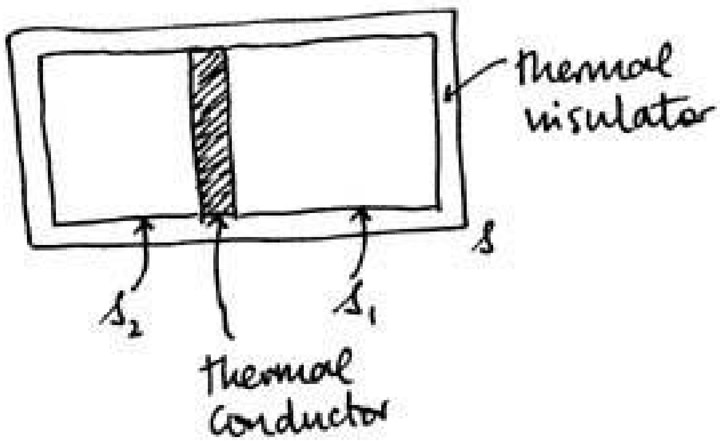
2 Systems 'talking' to one another

big new concept idea

5

Consider a big system $\mathcal{S}$
composed of $\mathcal{S}_1$ and $\mathcal{S}_2$, smaller {sub-} systems

Let $\mathcal{S}$ be closed
but allow $\mathcal{S}_1$ and $\mathcal{S}_2$ to exchange energy
(but not particles!) $\Rightarrow$ $\mathcal{S}_1, \mathcal{S}_2$ in <u>thermal contact</u>



* Basic idea: the most probable configuration
(way of distributing $U = U_1 + U_2$)
is the one with the biggest degeneracy

* Preview: We will define the <u>entropy</u> as

$$\sigma(N, U) = \log g(N, U)$$

and we will use knowledge of this and
energy U to <u>define</u> what we mean by
temperature!

jan14 6

First Example – our friend the spin system

How might energy be interchanged?

We have

$\mathcal{S}_1$: N_1 particles, energy U_1

$N_{1\uparrow}$ and $N_{1\downarrow}$ $\Rightarrow$ $2s_1 = N_{1\uparrow} - N_{1\downarrow}$

$\mathcal{S}_2$: N_2 particles, energy U_2,

$N_{2\uparrow}$ and $N_{2\downarrow}$ $\Rightarrow$ $2s_2 = N_{2\uparrow} - N_{2\downarrow}$

* N_1, N_2, $U = U_1 + U_2$ are fixed

(from the way we set up the problem)

but

s_1, s_2, $U_1 - U_2$ can vary!

- In our system, if $\uparrow$ and $\downarrow$ have the same energy the analysis is very boring, no energy can change.

But we learned last week that when a $\vec{B}$ field is on,

$U_1 = -2mB\, s_1$ for a system of N_1 spins

We can also write, in exactly the same way,

$U_2 = -2mB\, s_2$.

So we can exchange energy here between $\mathcal{S}_1$ and $\mathcal{S}_2$ in a $\vec{B}$-field by (say) flipping ~~some~~ n spins $\downarrow$ to $\uparrow$ in $\mathcal{S}_1$ and simultaneously flipping n spins $\uparrow$ to $\downarrow$ in $\mathcal{S}_2$!

• Let's find the degeneracy for a given N, U for the whole system.

$$g(N, s) = ?$$

Suppose we specify s_1 (N_1 is fixed).

This is enough to tell us U_1.

Then we also need s_2 (N_2 is fixed).

We can write $s_2 = s - s_1$ because $s_1 + s_2 = s$

So we should pick an s_1 and write

$$g_1(N_1, s_1)\; g_2(N_2, s - s_1)$$

fixed

varies

For the whole system we need to $\sum_{s_1}$

$$\Rightarrow \boxed{g(N, s) = \sum_{s_1} g_1(N_1, s_1)\, g_2(N_2, s - s_1)}$$

(Range of summation? $-\frac{1}{2}N_1$ to $+\frac{1}{2}N_1$)

* The most probable configuration will again have a very large degeneracy (as for the sole spin system) and the width of the peak again small

$\Rightarrow$ let's use the continuous approx. again