

Paul Martin - Basics

Physicists - sometimes need to model interacting many-body systems.  
 - following energy is helpful.

$$E_{kin} = \sum_{i=1}^N \frac{1}{2} m_i v_i^2$$

But  $\frac{dv}{dt} = F/m$ , so need to understand the forces acting.

eg.  $F_1 = \frac{q_1 q_2}{4\pi\epsilon_0 r_{12}^2} = -F_2$  Coulomb force.  $1 \leftrightarrow 2$

- displacement vector.

For a moment think of this as a force field created by  $q_2$  acting on  $q_1$ .

Conservative  $\Rightarrow F = -\nabla\phi$ , some  $\phi$ .

$\phi(r)$  is part of potential energy of  $m_1$ .

$$E_1 = \frac{1}{2} m_1 v_1^2 + \phi_1$$

So  $E$  depends on velocities & positions of all atoms in system.

We'll never keep track, prefer to know <sup>bulk</sup> averaged behaviour.

Call inaccessible complete microscopic specification "microstate" =  $\sigma$ . - encodes all v's & pos's.

For each  $\sigma$ , we know, in principle,  $E(\sigma)$

Ask: what is probability  $P(\sigma)$  of finding system in state  $\sigma$  at a given instant?

Expected value of bulk obs.

$$\langle O \rangle = \sum_{\sigma} O(\sigma) P(\sigma)$$

↑  
exp. value

But what is  $O(\sigma)$ ?

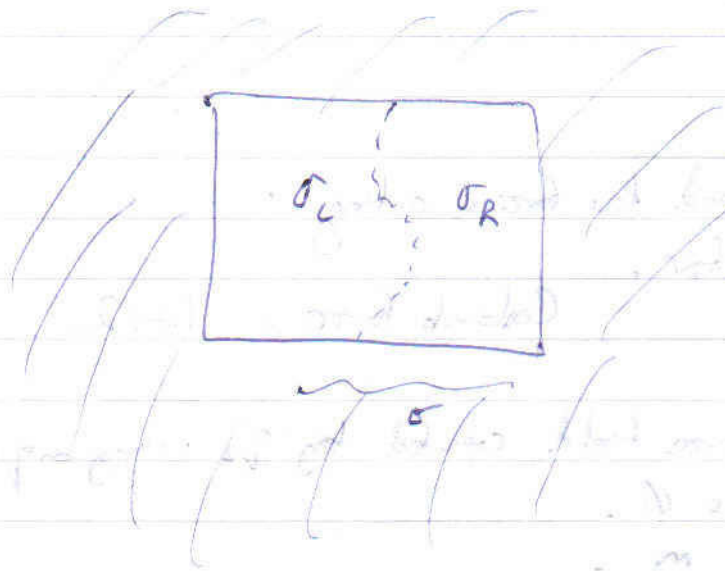
Intensive: doesn't grow.

Can Choose  $\sigma$

If all we know is the total energy  $E$ ,  $P(\sigma) = \begin{cases} 0 & E(\sigma) \neq E \\ 1/N_E & E(\sigma) = E \end{cases}$

We can't isolate a realistic system, so can't fix  $E$ , but will just assume  $P(\sigma) = P(E(\sigma))$ .

So what is this function?



$\sigma_L, \sigma_R$  indpt.  $P(\sigma) = P(\sigma_L) P(\sigma_R)$ . Can get energy from either side.

Meanwhile  $E = E_L + E_R + E_{\text{interaction}}$

$\rightarrow E \approx E_L + E_R$  (geometry). negligible, "only a line"

The L, R - m systems will each have their own energy probability function.

$$P(E_L + E_R) = P_L(E_L) P_R(E_R)$$

$$E_L, E_R \text{ indpt. , so } \frac{\partial P(E_L + E_R)}{\partial E_L} = \frac{\partial P(E_L + E_R)}{\partial E_R}$$

$$\frac{P'_L(E_L)}{P_L(E_L)} = \frac{P'_R(E_R)}{P_R(E_R)} = \underline{\underline{-\beta}} \text{ of wave equation.}$$

Write as  $-\beta$ , as must be constant.  
"const of separation"

$P_L(E_L) = -\beta P_L(E_L)$

$\therefore P(E) = C \exp(-\beta E)$

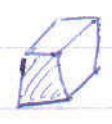
C fixed by  $\sum_{\sigma} P(E(\sigma)) = 1$

$\beta$  is only thing connecting subsystems

$Z(\beta) = \sum_{\sigma} \exp(-\beta E(\sigma))$  (inverse) temperature

"zustatensumme" (Boltzmann) is partition function

$P(E) = \frac{\exp(-\beta E)}{Z}$



Realistic systems even with no kinetics - absorb into  $\beta$

$Z$  is "just" a normalising factor

$\frac{d \ln Z}{d\beta} = -\frac{1}{Z} \sum_{\sigma} E(\sigma) \exp(-\beta E(\sigma)) = \text{expected energy}$

"internal energy"

$\frac{1}{N}$  per energy density  $U$

so its analysis contains physics



Suppose  $E: S \rightarrow \pm N$  (quantised).

Then  $Z$  poly. in  $\exp(\mp \beta)$ .

Only analytic structure is zeros.

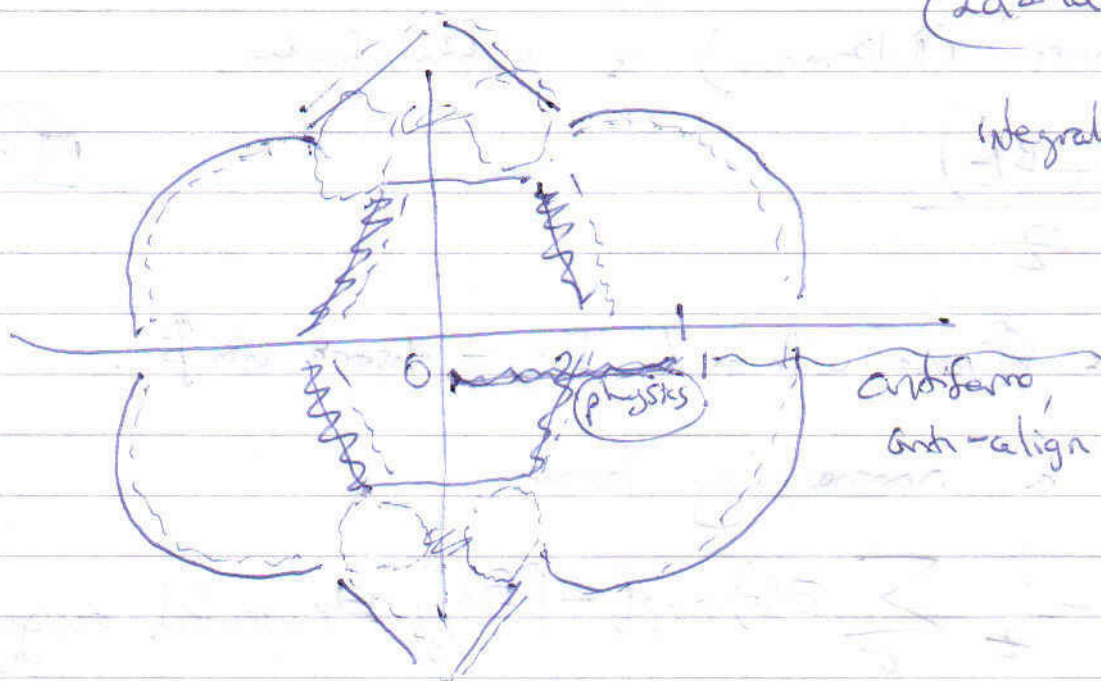
Descartes rule of signs

2-state Potts model for a <sup>cube</sup> ~~arbitrary~~ graph

3-d Ising model  
not integrable

(2d & 1d are integrable)

integrable  $\rightarrow$  enough symms  $\rightarrow$   
closed  
family of p.m.  
even for large  $N$ .



Qn What does this tell us?

Specific heat tells us the r.o.c. of internal energy with Temp.  
(or in practice, other way round):

$$S = \frac{\partial}{\partial \beta} \left( \frac{1}{N} \ln Z \right)$$

$$x = e^{\beta}$$

$$Z = \prod_j (x - x_j)$$

Integ. means  
knowing  $x_j$ 's.

$$\frac{\partial \left( \frac{1}{N} \ln Z \right)}{\partial \beta} = \frac{x}{N} \sum_j \frac{1}{x - x_j}$$

- get a (large) contribution from each zero,  $x \rightarrow 0$ ,  $\frac{1}{x} \rightarrow \infty$  gets large.

eg water, 2 phase transitions, use TL algebra.