

## A sketch of the statistical formalism for (emergent) phases

Charles Radin

- 1) *One defines a set  $X$  each point of which represents an infinite system of similar components.*  
Examples: A configuration of infinitely many unit cubes in  $\mathbb{R}^3$ ; a simple graph on infinitely many nodes, ...
- 2) *There are projections of each point in  $X$  onto 'finite subsystems' labelled by  $v$ .*  
Examples: Those cubes intersecting the ball centered at the origin of  $\mathbb{R}^3$  and radius  $v$ ; the subgraph induced by the nodes in  $v = \{1, 2, \dots, |v|\}, \dots$
- 3) *One chooses a few 'competing constraints'  $\epsilon$ .*  
Examples: Cube configurations with given volume fraction and given density of 'energy of interaction'; graphs with given edge and triangle densities, ...  
The set of possible vector values of  $\epsilon$  constitutes a constraint ('phase') space  $\mathcal{Y}$ , the boundary of which obviously corresponds to extrema of the constraints.
- 4) *One computes the number or volume  $Z_v(\epsilon)$  of constrained projected configurations, and its exponential rate of growth  $s(\epsilon) = \lim_{|v| \rightarrow \infty} (1/|v|) \log[Z_v(\epsilon)]$ .*  
(I've cheated by leaving out the step of thickening the constraints by  $\alpha$  and then taking  $\alpha \rightarrow 0$  after the limit in  $v$ .)
- 5) *There is a simple real valued function  $R$  on a (relevant, 'probabilistic') space  $\mathcal{F}_\epsilon$  such that  $s(\epsilon) = R(\mu_\epsilon)$  for one or more 'equilibrium states'  $\mu_\epsilon$  in  $\mathcal{F}_\epsilon$ . The  $\mu_\epsilon$  are characterized alternatively by (local) DLR equations, or as maximizers of  $R(\mu)$  among all  $\mu$  in  $\mathcal{F}_\epsilon$ .*  
(The  $\mu_\epsilon$  give a much richer picture of the system than the function  $s(\epsilon)$ .)

### Notes on the above

- i) Both characterizations in 5) of equilibrium states  $\mu_\epsilon$  were proven, for stat mech 'on lattices', in the 1960's. However for more realistic models, such as particles or cubes in a continuum such as  $\mathbb{R}^3$ , the DLR characterization of  $\mu_\epsilon$  was proven by Dobrushin and Lanford/Ruelle around 1969 but I don't believe the variational characterization was ever proven for such systems. For graphs the opposite is true: the variational characterization is proven but I don't think there is any analogue of the DLR characterization of the entropy maximizers  $\mu_\epsilon$ .
- ii) A simplified version of the Gibbs phase rule, unproven except in specific examples, states: 'Except for a set of constraints  $\epsilon$  of lower dimension,  $s(\epsilon)$  is real analytic at  $\epsilon$ .' The main point of the formalism: There exist simply stated examples (e.g. 'hard spheres') with multiple phases, i.e. for which the region  $\mathcal{A} \subset \mathcal{Y}$  of analyticity of  $s(\epsilon)$  is not connected.
- iii) The formalism 1) – 5) seems to be easier to develop/analyze in graphs than in stat mech. In particular the  $\mu_\epsilon$  are simple enough to 'understand' (multipodal) in graph models.
- iv) Note that for stat mech one can start in the grand canonical ensemble and derive the characterizations of 5) using the Legendre transform, but this does not work for graphs; the grand canonical ensemble loses information, and is misleading, for graphs.
- v) A large deviations principle can be useful to derive the variational characterization of 5) but is not necessary; the variational characterization was first developed in lattice stat mech by Ruelle (1965, 1967) without an underlying large deviations principle, though this path was later derived in the 1980's.

### Some questions

- a) Do we want to say that the system of noninteracting particles forms an emergent 'phase'?
- b) Why can material phases be determined by so few parameters?

D. Ruelle: J. Math. Phys. 6 (1965) 201-220; Commun. math. Phys. 5 (1967) 324-329

O.E. Lanford and D. Ruelle: Commun. math. Phys. 13 (1969) 194-215