Lecture 3

The main goal of this lecture is to prove Prop. 2.2 (Prop 2 of lecture 2). The secondary goal is to discuss the place of this result relative to the original goal of proving that grand canonical ensembles constructed from potentials that are more realistic than the mean field theory interaction also have "liquid-to-gas" phase transitions. Very few continuum particle systems in the continuum are rigorously known to have such phase transitions.

We begin with a technical Lemma 1 which encapsulates a principle due to Laplace and then give the proof of Proposition 2.1. Notice the step marked with exclamation point in this proof because we will re-use the same principle, which is to express a two body interaction as a mixture of external fields.

Lemma 1 (Laplace) Let S be a continuous function on $\mathbb{R}^n$ which has a unique global minimum at x_0. Furthermore $\int e^{-S} dx$ is finite and $\{x : S(x) \leq S(x_0) + 1\}$ is compact. Then

$$\lim_{t \to \infty} \frac{1}{(f=1)} \int e^{-tS} f \, dx = f(x_0)$$

for any bounded continuous f.

Proof Consider

$$M_\epsilon = \{x : S(x) \leq S(x_0) + \epsilon\}$$

For $\epsilon > 0$ it contains $\{x : S(x) < S(x_0) + \epsilon\}$ which is open because f is continuous. Therefore

$$\int_{M_\epsilon} e^{-S} dx \neq 0, \qquad \epsilon > 0.$$

If U is an open set containing x_0 then $U^c \cap M_1$ is compact so S has a minimum on $U^c \cap M_1$ which cannot equal x_0 so there is $\epsilon > 0$ such that

$$S(x) \geq S(x_0) + \epsilon \qquad x \notin U$$

We can, WLOG, assume $S(x_0) = 0$

Let

$$I_t(E, f) = \int_E e^{-tS} f \, dx, \qquad E \subset \mathbb{R}^n$$

Then

$$I_t(U^c, f) \leq \|f\|_\infty \, e^{-(t-1)\epsilon} \int e^{-S} dx$$

$$I_t(\mathbb{R}^n, 1) \geq I_t(M_{\epsilon/2}, 1)$$

$$\geq e^{-(t-1)\epsilon/2} \int_{M_{\epsilon/2}} e^{-S} dx$$

so

$$\frac{I_t(U^c, f)}{I_t(\mathbb{R}, 1)} \longrightarrow 0 \quad \text{as } t \to \infty \qquad \text{(a)}$$

$$\frac{I_t(U, 1)}{I_t(\mathbb{R}, 1)} \longrightarrow 1 \qquad \text{(b)}$$

Let $\epsilon > 0$. Choose U s.t.
$|f(x) - f(x_0)| < \epsilon$ for $x \in U$.

Then

$$\frac{I_t(\mathbb{R}, f)}{I_t(\mathbb{R}, 1)} \overset{(a)}{=} \frac{I_t(U, f)}{I_t(\mathbb{R}, 1)} + o(t)$$

$$\leq (f(x_0) + \epsilon) \underbrace{\frac{I_t(U, 1)}{I_t(\mathbb{R}, 1)}}_{\to 1 \text{ by (b)}} + o(t)$$

Likewise a lower bound in terms of $f(x_0) - \epsilon$. ∎

Proof of Proposition 2.2 Let $F = \mathbb{1}_{\underline{N}_X = \underline{n}}$

$$\langle F \rangle_{MFT,\Lambda} = \frac{1}{(F=1)} \sum_{n \in \Omega} z^{\underline{n}} e^{-H} F$$

$$= \frac{1}{(F=1)} \sum_{n \in \Omega} z^{\underline{n}} e^{\alpha \frac{N^2}{2}} F \qquad \alpha = \frac{\beta}{|\Lambda|_1}$$

$$= \frac{1}{(F=1)} \int \sum_{n \in \Omega} z^{\underline{n}} e^{\phi N} F \, e^{-\phi^2/2\alpha} \, d\phi$$

Let

$$\langle F \rangle_{\phi,\Lambda} = \frac{\sum z^{\underline{n}} e^{\phi N} F}{\sum z^{\underline{n}} e^{\phi N}} \qquad \text{Bernoulli}\,(1:ze^{\phi})$$

Now

$$\sum_{\underline{n} \in \Omega} z^{\underline{n}} e^{\phi N} = \sum (ze^{\phi})^{\underline{n}} = (1+ze^{\phi})^{|\Lambda|_1}$$

$$\langle F \rangle_{\phi,\Lambda} = \langle F \rangle_{\phi,X}$$

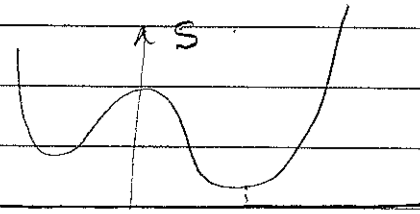
Then

$$\langle F \rangle_{MFT,\Lambda} = \frac{1}{(F=1)} \int (1+ze^{\phi})^{|\Lambda|_1} \langle F \rangle_{\phi,X} \, e^{-\phi^2/2\alpha} \, d\phi$$

$$= \frac{1}{(F=1)} \int e^{-|\Lambda|_1 S(\phi)} \langle F \rangle_{\phi,X} \, d\phi$$

Now take ∞ vol limit

$|\Lambda|_1 \to \infty$.



$\phi \sim \phi \in M_0$

$|M_0| = 1$

in this picture

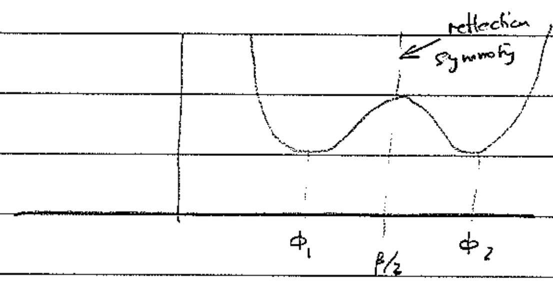
If (z,β) are such that S has a unique global minimum ϕ then Lemma 1 and our choice of F implies

$$\langle F \rangle_{MFT,\Lambda} \xrightarrow[|\Lambda|\nearrow\infty]{} \langle F \rangle_{\phi, X}$$

$$= \mathbb{P}_{\text{Bernoulli}}\{\underline{N}_X = n\}$$

<u>Claim</u>: Analysis of $S(\phi)$ shows that $S(\phi)$ has a unique global minimum if $\beta \le 4$ or if $ze^{\beta/2} \neq 1$.

If $\beta > 4$ and $ze^{\beta/2} = 1$ Lemma 2 (below) implies there are two global minima related by symmetry



With the symmetry it is trivial to modify Lemma 1 to finish case (2 phase).

∎

The claim is not fully proved in these notes but see the picture after Lemma 2.

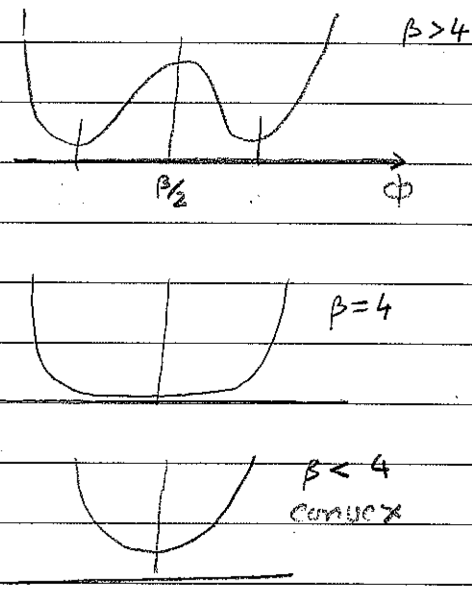
Lemma 2

For $(\beta, z) \in \{ z e^{\beta/2} = 1 \}$

$$S(\phi) = \frac{\eta^2}{2\beta} - \log\left(e^{-\eta/2} + e^{\eta/2}\right) + C_{\beta z}$$

$$\eta = \phi - \beta/2$$

There are two global minima $\phi = \beta/2 \pm \eta_c$ when $\beta > 4$, otherwise there is one global minimum.



Proof Let $\phi = \zeta + \eta$

$\log(1 + z e^{\phi})$

$$= \log\left(1 + z e^{\zeta} e^{\eta}\right)$$

Choose ζ so that $\boxed{z e^{\zeta} = 1}$

$$= \log\left(1 + e^{\eta}\right) = \log e^{\eta/2}\left(e^{-\eta/2} + e^{\eta/2}\right)$$

$$= \eta/2 + \log\left(e^{-\eta/2} + e^{\eta/2}\right)$$

Also $\displaystyle \frac{\phi^2}{2\beta} = \frac{(\zeta+\eta)^2}{2\beta} = \frac{\zeta^2}{2\beta} + \frac{\zeta\eta}{\beta} + \frac{\eta^2}{2\beta}$

so

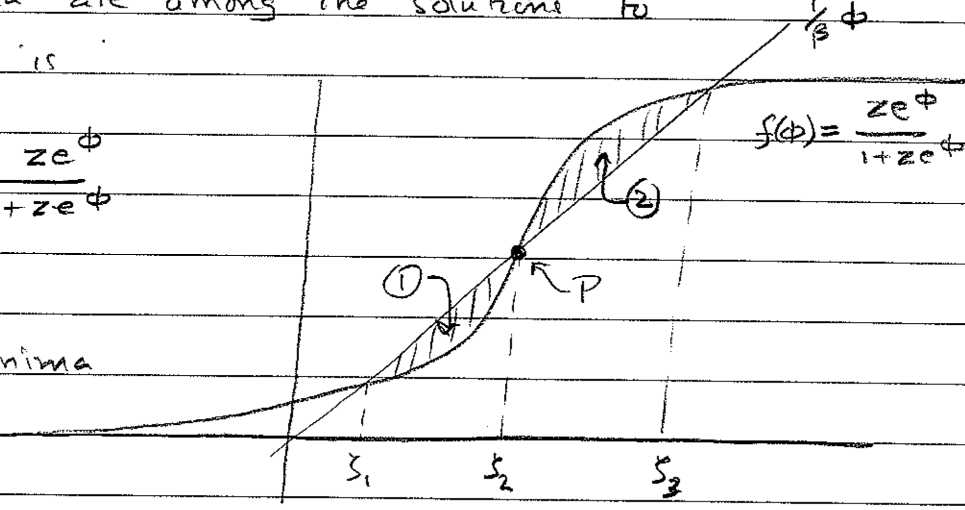
$$S(\phi) = \frac{\zeta^2}{2\beta} + \left(\frac{\zeta}{\beta} - \frac{1}{2}\right)\eta + \frac{\eta^2}{2\beta} - \log\left(e^{-\eta/2} + e^{\eta/2}\right)$$

If $\boxed{\zeta/\beta = \frac{1}{2}}$ then we have the formula for $S(\phi)$ claimed in Lemma.
If $(\beta, z) \in \{ z e^{\beta/2} = 1 \}$ then we can simultaneously solve $\zeta/\beta = 1/2$ and $z e^{\zeta} = 1$ as required. It is easy to check convexity iff $\beta \leq 4$. ∎

Graphical Interpretation

The global minima are among the solutions to $dS/d\phi = 0$ which is

$$\frac{1}{\beta}\,\phi = \frac{ze^{\phi}}{1+ze^{\phi}}$$



ζ_2 is a maximum

ζ_1, ζ_3 are local minima

$$S(\zeta_1) = S(\zeta_2) - \text{area } ①$$
$$S(\zeta_3) = S(\zeta_2) - \text{area } ②$$

For two global minima the shaded areas must be equal.

When P is the point of inflexion of $f(\phi)$ the two areas are equal because f is odd about P.

To fully prove case (1 phase) of Proposition 2·2 we have to show that the shaded areas are not equal if ζ_2 is not a point of inflexion.

Discussion

Let V be built from 2-body potential

$$U(x,y) = \infty \quad \text{if} \quad |x-y| \leq 1$$
$$= -\ell^{-d} f\left(\frac{\|x-y\|}{\ell}\right) \quad \text{else}$$

where $f \geq 0$ and $\int f\,dx = 1$.

Kac began the study of $\ell \to \infty$ in 1959

Lebowitz - Penrose 1966 proved that the Kac limit of the pressure is the mean field theory pressure for particles in the continuum with hard core + attractive potential

Lebowitz Mazel Presutti 1999 proved existence of phase transitions near the Kac limit for particles in the continuum with attractive potential and a 4-body repulsion. The latter is un-natural. It is a very interesting open problem to prove that (hard core + 2-body attractive) systems have phase transitions near the Kac limit.

This is interesting because in almost no cases do we have proofs that particle systems in the continuum exhibit phase transitions.

Problems

(1) Show that when $(\beta, z) \in \{z e^{\beta/2} = 1\}$ the probabily of any configuration in the MFT model is invariant under $\{ n_B \leftrightarrow 1 - n_B \ \forall B \}$

(2) Write (lattice gas) as a standard Ising model by $n_B = 1 \iff \text{spin}_B = \frac{1}{2}$
$n_B = -1 \iff \text{spin}_B = -\frac{1}{2}$.

(3) Discuss the connection of Proposition I with the de Finetti Theorem on p 269 of [Durrett]

(4) Omit the step where we introduce the blocks $\mathcal{B}(\Lambda)$ and consider the grand canonical ensemble with

$$V(x) = -\frac{\beta}{|\Lambda|} \frac{N^2(x)}{2}.$$

Notice there is no hard core condition
Apply the same idea,

$$e^{-\alpha \frac{N^2}{2}} = \frac{1}{\sqrt{2\pi}} \int e^{\phi N} e^{-\phi^2/2\alpha} \, d\phi$$

What is S in this case. What goes wrong and why did introducing the condition $V = \infty$ if any $N(B) > 1$ avoid this problem?