Equilibrium States of Interacting Particle Systems

Diana Conache

Technische Universität München

A Talk in the Framework of 
”Konstanz Women in Mathematics”
February 2016
1. Basics of Statistical Mechanics
2. The Existence Problem for Gibbs Fields
3. The Uniqueness Problem for Gibbs Fields
4. Classical Systems in Continuum
Motivation

A particular aim of statistical mechanics is to study the macroscopic behaviour of a system, knowing the behaviour of the microscopic states \( x = (x_\ell)_{\ell \in \mathbb{Z}^d} \) given by collections of \( \Xi \)-valued random variables.

The equilibrium states of the system are heuristically described by probability measures of the form

\[
\mu = \frac{1}{Z} e^{-\beta H(x)} \, dx.
\]

However, for an infinite configuration \( x = (x_\ell)_{\ell \in \mathbb{Z}^d} \), the Hamiltonian \( H(x) \) is not well-defined and thus, the definition of \( \mu \) makes no sense.
Dobrushin-Lanford-Ruelle Approach

Idea: construct probability measures $\mu$ on $(\Xi)^{\mathbb{Z}^d}$ with prescribed conditional probabilities given by the family of stochastic kernels

$$\pi_L(A|y) = \frac{1}{Z_L(y)} \int_{(\Xi)^{\mathbb{Z}^d}} 1_A(x) \exp \left\{ -\beta H_L(x_L|y) \right\} \otimes_{\ell \in L} dx \otimes_{\ell' \in L^c} \delta_{y\ell'}.$$ 

Main problems (since 1970):

- existence (Dobrushin, Ruelle, ...);
- uniqueness/ non-uniqueness $\implies$ phase transitions
  - finite or compact $\Xi$ (Dobrushin, Ruelle, ...);
  - non-compact $\Xi$ (Lebowitz and Presutti-for a particular model; Dobrushin and Pechersky (1983) - in the general case).
Phase Transitions - The 2D-Ising Model

• the configuration space is \( X := \{-1, +1\}^{\mathbb{Z}^2} \).

• the local energy of \( x \) with boundary condition \( y \)

\[
H_L(x_L | y) := J \sum_{\ell \sim \ell', \ell, \ell' \in L} x_\ell x_{\ell'} + J \sum_{\ell \sim \ell', \ell \in L, \ell' \not\in L} x_\ell y_{\ell'} + h \sum_{\ell \in L} x_\ell
\]

• the system of conditional distributions \( \Pi = \{\pi_L(\cdot | y)\}_{L \in \mathbb{Z}^2, y \in X} \), where

\[
\pi_\beta^L(B | y) := \frac{1}{Z_\beta^L} \int_{X_L} 1_B(x_L \times y_L^c) \exp \{-\beta H_L(x_L | y)\} \nu_L(dx_L)
\]

**Theorem**

For all \( \beta \) large enough and \( h = 0 \), there exist two pure limit Gibbs distributions for the 2D ferromagnetic \((J > 0)\) Ising model.
Outline

1. Basics of Statistical Mechanics
2. The Existence Problem for Gibbs Fields
3. The Uniqueness Problem for Gibbs Fields
4. Classical Systems in Continuum
Main question: Given a specification $\Pi$, does there exist a Gibbs measure consistent with $\Pi$?

Strategy: Introduce a topology on $\mathcal{P}(X)$, pick a boundary condition $y \in X$ and show that

(I) the net $\{\pi_L(\cdot|y)\}_L$ has a cluster point with respect to the chosen topology;

(II) each cluster point of $\{\pi_L(\cdot|y)\}_L$ is consistent with $\Pi$.

Trick: Choosing the best-suited topology on $\mathcal{P}(X)$, which in this case turns out to be the topology of local convergence.
Dobrushin’s Existence Criterion

If the one-point specification associated to $\Pi$ satisfies the condition below, then (I) is satisfied. For (II) some continuity assumption is also needed.

**Compactness Condition:** There exist a compact function $h : \Xi \to \overline{\mathbb{R}}_+$ and nonnegative constants $C$ and $I_{\ell\ell'}$, $\ell \neq \ell'$ such that

(i) The matrix $I = (I_{\ell\ell'})_{\ell, \ell' \in V}$ satisfies

$$\|I\|_0 := \sup_{\ell} \sum_{\ell' \neq \ell} I_{\ell\ell'} < 1.$$ 

(ii) For all $\ell \in V$ and $y \in X$

$$\int_X h(x_\ell) \pi_\ell(dx_\ell|y) \leq C + \sum_{\ell' \neq \ell} I_{\ell\ell'} h(x_{\ell'}).$$
Outline

1. Basics of Statistical Mechanics
2. The Existence Problem for Gibbs Fields
3. The Uniqueness Problem for Gibbs Fields
4. Classical Systems in Continuum
Approaches in Solving the Uniqueness Problem

- Dobrushin classical criterion, Dobrushin-Pechersky, Dobrushin-Shlosman;
- exponential decay of correlations;
- exponential relaxation of the corresponding Glauber dynamics, expressed by means of the log-Sobolev and Poincaré inequalities for $\pi(dx|y)$;
- Ruelle’s superstability method.

Most methods work only in the case of a compact spin space. We will focus on the Dobrushin-Pechersky criterion, which can be applied also to more general spin spaces.
Contraction Condition

Assume that $\pi$ satisfies

$$d(\pi^x_\ell, \pi^y_\ell) \leq \sum_{\ell' \in \partial \ell} \kappa_{\ell\ell'} 1_{(x_{\ell'}, y_{\ell'})},$$

(CC)

for all $\ell \in V$ and $x, y \in X_\ell(h, K)$, where $\kappa = (\kappa_{\ell\ell'})_{\ell, \ell' \in V}$ has positive entries and null diagonal such that

$$\bar{\kappa} := \sup_{\ell \in V} \sum_{\ell' \in \partial \ell} \kappa_{\ell\ell'} < 1.$$

For a constant $K > 0$, $\ell \in V$ and a measurable function $h : \Xi \to \mathbb{R}_+ := [0, +\infty)$, we set

$$X_\ell(h, K) = \{x \in X : h(x_\ell) \leq K \text{ for all } \ell \in \partial \ell\}.$$
Moreover, suppose $h$ satisfies the following integrability condition

$$
\pi^x_\ell(h) \leq 1 + \sum_{\ell' \in \partial \ell} c_{\ell \ell'} h(x_{\ell'}),
$$

(IC)

for all $\ell \in V$ and $x \in X$, where $c = (c_{\ell \ell'})_{\ell, \ell' \in V}$ has positive entries and null diagonal such that

$$
\bar{c} := \sup_{\ell \in V} \sum_{\ell' \in \partial \ell} c_{\ell \ell'} < \mathcal{C}(\text{graph}) < 1.
$$

We introduce the set of tempered measures $\mathcal{M}(\pi, h)$ consisting of all measures $\mu \in \mathcal{M}(\pi)$ for which

$$
\sup_{\ell} \int_X h(x_{\ell}) \mu(dx) < \infty.
$$
The Uniqueness Result

**Theorem**

For each $K > K_*(graph)$ and $\pi \in \Pi(h, K, \kappa, c)$, the set $\mathcal{M}(\pi, h)$ contains at most one element.

The proof of the theorem follows immediately from

**Lemma**

Let $\mu_1, \mu_2 \in \mathcal{M}(\pi, h)$ and $\nu \in \mathcal{C}(\mu_1, \mu_2)$ such that

$$\gamma(\nu) := \sup_{\ell \in \mathcal{V}} \int_X \int_X \mathbb{1}_{x_{\ell} \neq x'_{\ell}} \nu(dx_1, dx_2) = 0.$$ 

Then $\mu_1 = \mu_2$. 
The Uniqueness Problem for Gibbs Fields

The Uniqueness Result

**Theorem**

For each $K > K^*_\text{graph}$ and $\pi \in \Pi(h, K, \kappa, c)$, the set $\mathcal{M}(\pi, h)$ contains at most one element.

The proof of the theorem follows immediately from

**Lemma**

Let $\mu_1, \mu_2 \in \mathcal{M}(\pi, h)$ and $\nu \in \mathcal{C}(\mu_1, \mu_2)$ such that

$$
\gamma(\nu) := \sup_{\ell \in \mathcal{V}} \int_X \int_X 1_{x_1^\ell \neq x_2^\ell} \nu(dx_1^1, dx_2^2) = 0.
$$

Then $\mu_1 = \mu_2$. 

Comparison with Dobrushin’s Classical Criterion

An earlier uniqueness result due to Dobrushin (1968), for $\Xi$ Polish, compact with $\rho$ a metric that makes $\Xi$ complete, requires that the following interdependence matrix be $\ell^\infty$–contractive, i.e.

$$D_{\ell\ell'} := \sup_{y^1, y^2 \in X} \left\{ \frac{W_\rho(\pi_{y^1}, \pi_{y^2})}{\rho(y^1, y^2)} \right\} < 1, \; \ell \neq \ell'.$$

Advantages of the DP approach:

- one needs to check the condition of weak dependence not for all boundary conditions (like here), but only for such $y \in X$ whose components $y_\ell$ lie in a certain ball in $\Xi$;
- it can also be applied for non-compact spins and for pair-potentials with more than quadratic growth.
The Uniqueness Problem for Gibbs Fields

Decay of Correlations for Gibbs measures

Theorem

Let $\pi$ and $K$ be as in the previous theorem and $\mathcal{M}(\pi, h)$ be nonempty, hence containing a single state $\mu$. Consider bounded functions $f, g : X \to \mathbb{R}_+$, such that $f$ is $\mathcal{B}(\Xi_{\ell_1})$-measurable and $g$ is $\mathcal{B}(\Xi_{\ell_2})$-measurable. Then there exist positive $C_K$ and $\alpha_K$, dependent on $K$ only, such that

$$|\text{Cov}_{\mu}(f; g)| \leq C_K \|f\|_\infty \|g\|_\infty \exp \left[ -\alpha_K \delta(\ell_1, \ell_2) \right], \quad \ell_1, \ell_2 \in L$$
Outline

1. Basics of Statistical Mechanics
2. The Existence Problem for Gibbs Fields
3. The Uniqueness Problem for Gibbs Fields
4. Classical Systems in Continuum
Configuration Spaces

- System of identical particles (or molecules of gas) in $\mathbb{R}^d$ interacting via a pair potential $V(x, y)$ with certain stability properties

$$H(\gamma) := \sum_{\{x, y\} \subset \gamma} V(x, y) \in \mathbb{R}, \ \gamma \in \Gamma$$

- $\mathbb{R}^d \ni x$ – position of each particle
- $\mathcal{B}_c(\mathbb{R}^d)$ - family of all bounded Borel sets in $\mathbb{R}^d$
- $\Gamma$ – configuration space consisting of all locally finite subsets $\gamma$ in $\mathbb{R}^d$

$$\Gamma := \left\{ \gamma \subset \mathbb{R}^d \left| |\gamma_\Lambda| < \infty, \ \forall \Lambda \in \mathcal{B}_c(\mathbb{R}^d) \right. \right\}$$

$|\gamma_\Lambda|$ is the number of points in $\gamma_\Lambda := \gamma \cap \Lambda$

- $\gamma$ is identified with the positive Radon measure $\sum_{x \in \gamma} \delta_x$
Poisson Measure

Poisson random point field $\pi_{z\sigma}$ on $\Gamma$ describes the state of an ideal gas

- $z > 0$ – chemical activity
- $\sigma(dx)$ – locally finite non-atomic measure on $\mathbb{R}^d$, $\sigma(\mathbb{R}^d) = \infty$,
- $\sigma$-Poisson measure $\lambda_{z\sigma}^\Lambda$ on $(\Gamma_\Lambda, \mathcal{B}(\Gamma_\Lambda))$
  \[
  \int_{\Gamma_\Lambda} F(\gamma_\Lambda) d\lambda_{z\sigma}(\gamma_\Lambda) := F(\{\emptyset\}) +
  \sum_{n \in \mathbb{N}} \frac{z^n}{n!} \int_{\Lambda^n} F(\{x_1, \ldots, x_n\}) d\sigma(x_1) \ldots d\sigma(x_n), \quad \forall F \in L^\infty(\Gamma_\Lambda)
  \]
- probability measure $\pi_{z\sigma}^\Lambda := e^{-z\sigma(\Lambda)} \lambda_{z\sigma}^\Lambda$ on $(\Gamma_\Lambda, \mathcal{B}(\Gamma_\Lambda))$
- Poisson measure $\pi_{z\sigma} \in \mathcal{P}(\Gamma)$ is the projective limit of $\pi_{z\sigma}^\Lambda$, i.e.
  \[
  \pi_{z\sigma} := \mathbb{P}_{\Lambda}^{-1} \circ \pi_{z\sigma}^\Lambda, \quad \Lambda \in \mathcal{B}_c(\mathbb{R}^d)
  \]
- Interpretation: for disjoint $(\Lambda_j)_{j=1}^N$, the variables $|\gamma_{\Lambda_j}|$ are mutually independent and distributed by the Poissonian law with $z\sigma(\Lambda_j)$
Local Gibbs States

- Interaction energy between $\gamma_\Lambda \in \Gamma_\Lambda$ and $\xi_{\Lambda^c} := \xi \cap \Lambda^c$
  \[
  W(\gamma_\Lambda|\xi) := \sum_{x \in \gamma_\Lambda, y \in \xi_{\Lambda^c}} V(x, y)
  \]

- Local Hamiltonians $H_\Lambda(\cdot|\xi) : \Gamma_\Lambda \to \mathbb{R}$
  \[
  H_\Lambda(\gamma_\Lambda|\xi) := H(\gamma_\Lambda) + W(\gamma_\Lambda|\xi), \quad \gamma_\Lambda \in \Gamma_\Lambda
  \]

- Partition function $1 < Z_\Lambda(\xi) \leq \infty$
  \[
  Z_\Lambda(\xi) := \int_{\Gamma_\Lambda} \exp \left\{ -\beta H_\Lambda(\gamma_\Lambda|\xi) \right\} d\lambda z\sigma(\gamma_\Lambda) = 1 + z +
  \]
  \[
  + \sum_{n \geq 2} \frac{z^n}{n!} \int_{\Lambda^n} \exp \left\{ -\beta H_\Lambda(\{x_1, \ldots, x_n\}|\xi) \right\} d\sigma(x_1) \cdots d\sigma(x_n) \geq 1
  \]

- Local Gibbs states $\mu_\Lambda(d\gamma_\Lambda|\xi)$ with boundary conditions $\xi \in \Gamma$
  is probability measures on $(\Gamma_\Lambda, \mathcal{B}(\Gamma_\Lambda))$ provided $Z_\Lambda(\xi) < \infty$
  \[
  \mu_\Lambda(d\gamma_\Lambda|\xi) := [Z_\Lambda(\xi)]^{-1} \exp \left\{ -\beta H_\Lambda(\gamma_\Lambda|\xi) \right\} \lambda z\sigma(d\gamma_\Lambda)
  \]
Strategies for Studying $\mu$

- **Stability Condition**: allows to construct $\mu \in \mathcal{G}$ at small $\beta$ and $z$ (by *cluster expansions* or *Kirkwood-Salsburg equation*; see Ruelle '69).

- **Ruelle’s Superstability**: proves existence at all $\beta$ and $z$ via *à-priori* bounds on *correlation functions* (i.e., certain moments) of Gibbs measures (see Ruelle '70). *Ruelle’s bound* on correlation functions $\Rightarrow$ convergence $\pi_{\Lambda_N}(d\gamma|\emptyset) \to \mu \in \mathcal{G}$ *locally setwise*. Highly nontrivial, combinatorial technique.

- **Dobrushin’s approach**: by reduction to *lattice systems* and use of *Dobrushin’s existence criterion* (1970)

- **Kondratiev, Pasurek, Röckner** develop an elementary technique of getting existence and *à-priori* bounds for $\mu \in \mathcal{G}^t$; its *conceptual difference* is a systematic use of (infinite dimensional) Stochastic Analysis.
Theorem

Under some assumptions on the pair potential $W$, for fixed $\beta$ and small enough $z$, the set of Gibbs measures is a singleton.

Strategy of proof: partition $\mathbb{R}^d = \bigcup_{k \in \mathbb{Z}^d} Q_{gk}$ by equal cubes centred at points $gk$

$$Q_{gk} := \left\{ x = (x^{(i)})_{i=1}^d \left| g \left( k^{(i)} - 1/2 \right) \leq x^{(i)} < g \left( k^{(i)} + 1/2 \right) \right. \right\},$$

with edge length $g := \delta/\sqrt{d}$ and diam$(Q_{gk}) = \delta$ and define an equivalent lattice model on $(\Gamma(\bar{Q}_0))^{\mathbb{Z}^d}$. Show then that in this new model, there exists at most one Gibbs measure. Then show that any Gibbs measure in the initial model corresponds to a Gibbs measure in the new lattice model.
Thank you for your attention!