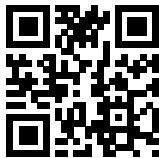


The liquid-vapor phase transition in a system with a finite but coarse-grained attraction

Ian Jauslin

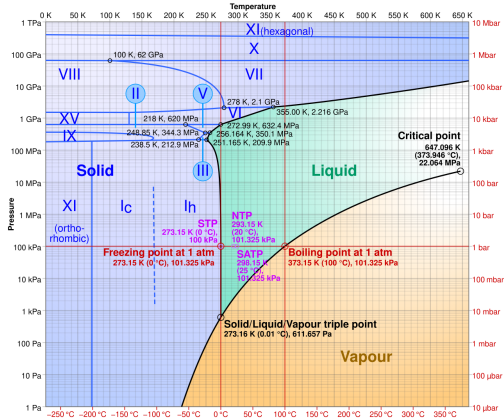
joint with Qidong He, Joel L. Lebowitz, Ron Peled



arXiv: 2510.24825

<http://ian.jauslin.org>

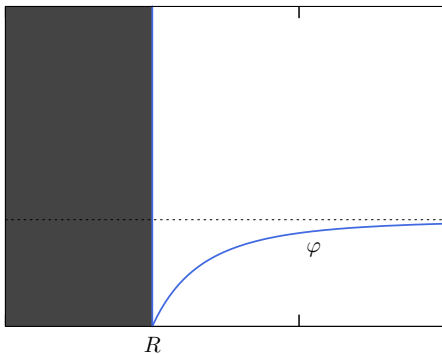
Phase diagram of water



© Cmglee, CC BY-SA 3.0

The Van der Waals model

- Model: interaction potential: **hard-core** plus **attractive** φ :



The Van der Waals equation of state

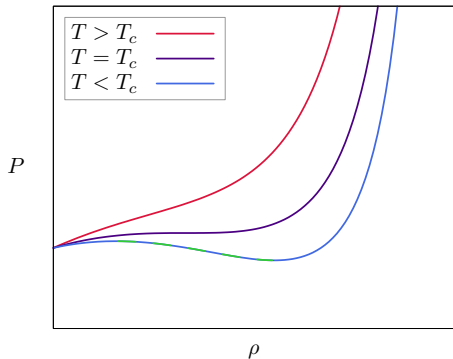
- Van der Waals: **heuristic** computation:

$$P(\rho) = \frac{T\rho}{1-\rho} + \frac{1}{2}\rho^2 \int dy \varphi(|y|)$$

where

- ▶ ρ : density
- ▶ P : pressure
- ▶ T : temperature

Pressure



- When the pressure is **decreasing**, the system is **unstable**. (Squeezing lowers the pressure!)

Free energy

- The free energy f solves

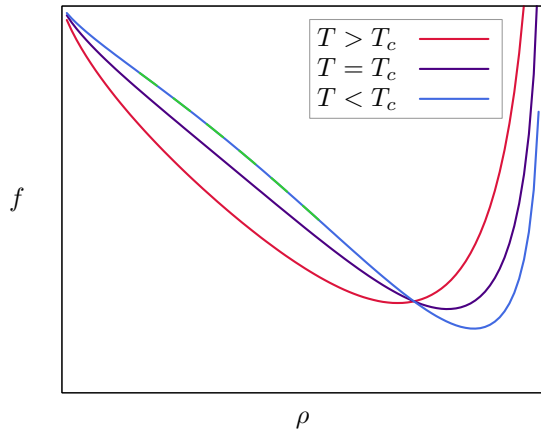
$$\frac{\partial^2 f}{\partial \rho^2} = \frac{1}{\rho} \frac{\partial P}{\partial \rho}$$

- Following Van der Waals,

$$f = T\rho \log \left(\frac{\rho e^{-1}}{1 - \rho} \right) + \frac{1}{2} \rho^2 \int_{|y|>R} dy \varphi(|y|)$$

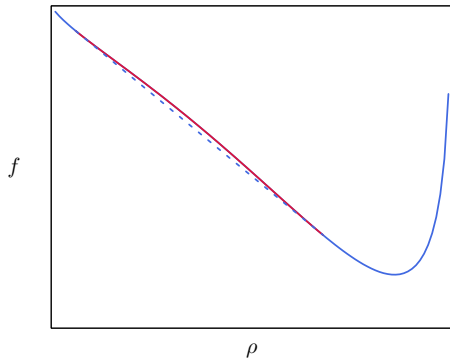
- The pressure is decreasing if and only if f is **concave**.

Free energy



Maxwell double tangent construction

- Idea: take the **convex envelope** of f :



The Lebowitz-Penrose theorem

- [Lebowitz, Penrose, 1966], [Kac, Uhlenbeck, Hemmer, 1963] Hard-core plus attractive interaction $\gamma^d \varphi(\gamma x)$.
- Take the limit $\gamma \rightarrow 0$.
- In other words, the attraction is of **infinite range** and **infinitely weak (mean-field)**.
- **Theorem** [LP66]: f_0 : free energy without the attraction, if $\gamma \rightarrow 0$,

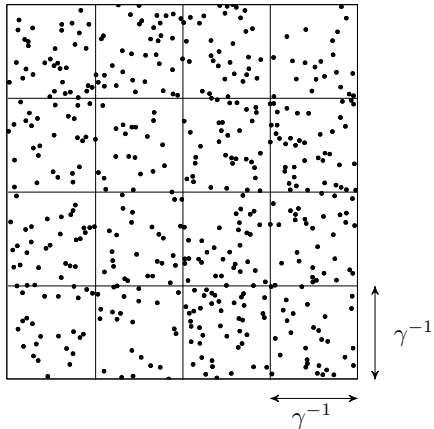
$$f(\rho) = \text{CE} \left(f_0(\rho) + \frac{1}{2} \rho^2 \int \varphi \right)$$

In particular, there is a **phase transition** when $f_0 + \frac{1}{2} \rho^2 \int \varphi$ is **not convex**.

Finite γ

- Open problem: existence of a phase transition for $0 < \gamma \ll 1$.
- [Lebowitz, Mazel, Presutti, 1999] [Presutti, 2009]: Proved a phase transition at $0 < \gamma \ll 1$ by adding a **four-body** long-range repulsion.
- Our result: prove a phase transition in a model with a **pair interaction**. The interaction we consider is a **coarse-grained** version of a more realistic interaction.

The Box model



The Box model

- We **coarse-grain** the attraction on mesoscopic boxes of size γ^{-1} .
- We ignore the repulsion **between** different boxes.
- In other words, the interaction becomes

$$u_\gamma(x - y) = \begin{cases} \text{hard core}(x - y) - J_1\gamma^d & \text{if } \text{Box}_\gamma(x) = \text{Box}_\gamma(y) \\ -J_2\gamma^d & \text{if } \text{Box}_\gamma(x) \text{ is next to } \text{Box}_\gamma(y) \\ 0 & \text{otherwise} \end{cases}$$

- The probability of a configuration x_1, \dots, x_N is proportional to

$$e^{-\beta \sum_{i < j} u_\gamma(x_i - x_j) + \beta \lambda N}.$$

λ : **chemical potential**.

The Box model as a spin model

- The box model is equivalent to a nearest-neighbor **spin** model on the lattice \mathbb{Z}^d , where each vertex of \mathbb{Z}^d corresponds to a **box**, and the spin value ρ_i corresponds to the **density** of particles in the box.
- The Hamiltonian for the spin model is

$$H = \gamma^{-d} \left(-\frac{1}{2} J_1 \sum_i \rho_i^2 - J_2 \sum_{i \sim j} \rho_i \rho_j + \sum_i f_\gamma(\rho_i) - \lambda \sum_i \rho_i \right)$$

where $f_\gamma(\rho)$ is the specific **free energy** for a system of **hard-core** particles in a box of size γ^{-1} .

The free energy in a box

- The free energy f_γ in a box with $N \equiv \rho\gamma^{-d}$ particles of radius R is

$$f_\gamma(\rho) := -\frac{1}{\beta\gamma^{-d}} \log \frac{1}{N!} \int_{([0,\gamma^{-1})^d)^N} dx_1 \cdots dx_N \prod_{i < j} \mathbb{1}_{|x_i - x_j| > 2R}$$

- (We can be more general and just assume that f_γ is the free energy for **any** system of particles in a box interacting via a **superstable** and **tempered** potential.)
- (Our result is actually even more general, and allows for a larger class of functions f_γ .)

Main result

- **Theorem:** If

$$f_0(\rho) - \frac{1}{2}(J_1 + 2dJ_2)\rho^2$$

- is **non-convex**, then there exists $\gamma_0 > 0$ such that for all $\gamma \leq \gamma_0$, there exists a chemical potential λ at which the box model admits two **distinct** translation invariant **Gibbs measures** that differ in their value of the **density**.
- Thus, in this case, there is a **first-order phase transition** at λ .
 - $f_0(\rho) = \lim_{\gamma \rightarrow 0} f_\gamma(\rho)$, so the condition for the existence of a phase transition is **the same** as for the Lebowitz-Penrose theorem.

The Dobrushin-Shlosman criterion

- [Dobrushin, Shlosman, 1981]
- Idea: if there are two **disjoint** intervals E_1, E_2 such that
 - ▶ $\mathbb{P}_\lambda(\rho_v \in E_1 \cup E_2)$ is large $\forall v$
 - ▶ $\mathbb{P}_\lambda(\rho_v \in E_1, \rho_w \in E_2)$ is small $\forall v, w$
 - ▶ for small λ , $\mathbb{P}_\lambda(\rho_v \in E_1)$ is large and, for large λ , $\mathbb{P}_\lambda(\rho_v \in E_2)$ is large

then there is an **intermediate** value of λ where two phases coexist, one favoring $\rho_v \in E_1$ and the other favoring $\rho_v \in E_2$.

Reflection positivity and chessboard estimate

- For any $f(\rho)$ and any reflection θ through an edge,

$$\mathbb{E}(f(\rho)f(\theta(\rho))) \geq 0.$$

- Suppose E is an **improbable** set of values for ρ_v . Take f to be $\mathbb{1}_E - \langle \mathbb{1}_E \rangle$:

$$\mathbb{P}(\rho_v \in E) \leq \mathbb{P}(\rho_v \in E, \theta(\rho)_v \in E)^{\frac{1}{2}}.$$

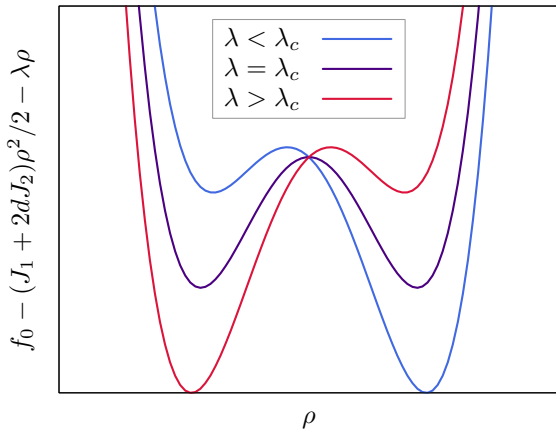
- Use more reflections to **spread the event** $\rho_v \in E$ to all vertices.

Ideas of the proof

- Idea: Use the **chessboard estimate** to prove the assumptions of the **Dobrushin-Shlosman** criterion.
- Reflection-positivity is a very **special** property, but it is central to the argument. Our proof thus **does not extend** to non-coarse-grained models.
- On the other hand, using the tools of reflection-positivity, the proof is relatively **easy**.
- Using the chessboard estimate, we get bounds in terms of **local** considerations, involving the minimization of

$$f_0(\rho) - \frac{1}{2}(J_1 + 2dJ_2)\rho^2 - \lambda\rho.$$

The Dobrushin-Shlosman criterion



Conclusion and outlook

- We have proved a **liquid-vapor** phase transition in a system with a **pair interaction**.
- However, our proof relies on **reflection positivity**, and requires the interaction to be simplified (**coarse-grained**).
- On the other hand, using reflection positivity makes the proof rather **easy**, so the box model serves as a good **toy model** for the liquid-vapor phase transition.
- Open problem: what about the more **realistic** interaction $\gamma^d \varphi(\gamma x)$? Can the coarse-graining be shown to be a good **approximation**? (This is what is done in [Presutti, 2009] in the presence of a 4-body repulsion.)