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Microstructures in one dimensional systems

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Microstructures thus appear on scales very small in macroscopic units yet very large microscopically.

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There is a good theory of the phenomenon in the context of variational problems for suitable energy or free energy functionals.

Stefan Müller and his school among the main contributors and I borrow an example from his lectures on elasticity:

Müller example.

Minimize the functional

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Both requests can be simultaneously met and the inf of $F(u)$ is 0:

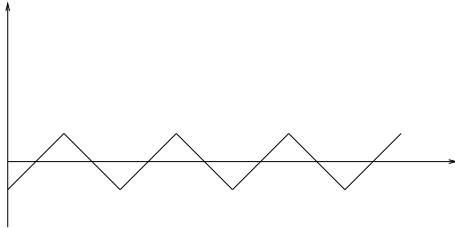


Figure: minimizing sequence: values between $\pm\epsilon$ with slope ± 1

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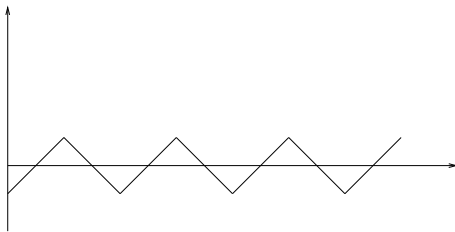


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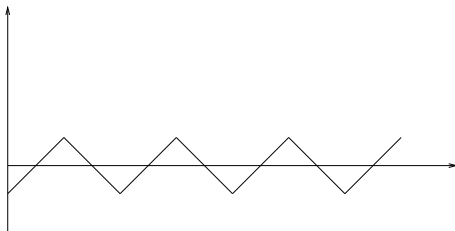


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The integral of u^2 is on “scale 1”, du/dx on an infinitesimal scale, the two scales are infinitely far apart and as a consequence the period of oscillations is infinitesimal.

Phase transitions.

The role of the two slopes in statistical mechanics is played by the two values of the density at phase transition.

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If we put in the box Λ a mass $\rho|\Lambda|$ of fluid with $\rho \in (\rho', \rho'')$, (“canonical constraint”) we do not see a homogeneous density ρ , but a density ρ' in a subset $\Lambda' \subset \Lambda$ and ρ'' in the complement.

The Ginzburg-Landau free energy functional.

Ginzburg-Landau's explanation of forbidden intervals.

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The free energy of a magnetization profile $u(x)$ in $\Lambda = [-L, L]$ is:

$$F_L(u) = \int_{-L}^L \left(u^2 - 1 \right)^2 + \left(\frac{du}{dx} \right)^2$$

The free energy when the total magnetization is m is:

$$f_L(m) := \frac{1}{2L} \inf \left\{ F(u) \mid \frac{1}{2L} \int_{-L}^L u = m \right\}$$

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In most of the space we see magnetization ± 1 .

Wulff shape versus microstructures.

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Going back to Müller example, $\int u^2$ plays the role of the long range forces and the ± 1 slopes correspond to the two pure phase densities ρ' and ρ'' .

Kac potentials

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The limit free energy in Kac systems is:

$$f_{\beta}^{\text{m.f.}}(\rho) = \phi_{\beta}^{**}(\rho), \quad \phi_{\beta}(\rho) = e(\rho) + f_{\beta}^{\text{s.r.}}(\rho)$$

where ϕ_{β}^{**} is the convexification of ϕ_{β} .

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The long range Hamiltonian is:

$$H_{\gamma}(q) = \int_{\mathbb{R}^d} e(J_{\gamma} * q), \quad J_{\gamma} * q(r) = \sum_{q_i \in q} J_{\gamma}(r, q_i)$$

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The free energy of $H_{\gamma} + H^{\text{s.r.}}$ in the limit $\gamma \rightarrow 0$ is $f_{\beta}^{\text{m.f.}}$.

Examples of Kac potentials.

Kac original model:

$e(\rho) = -\alpha \frac{\rho^2}{2}$, $\alpha > 0$; the short range force is the hard core interaction.

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LMP model (Lebowitz, Mazel, Presutti):

$$e(\rho) = -\frac{\rho^2}{2} + \frac{\rho^4}{4!}, \quad H^{\text{s.r.}} = 0.$$

It has phase transitions when $\gamma > 0$ is small

The two models are not good for microstructures because:

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in LMP the short range forces do not produce phase transitions.

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We want:

- ▶ $f_{\beta}^{\text{s.r.}}(\rho)$ linear (i.e. with a phase transition) in (ρ', ρ'')
- ▶ $\phi_{\beta}^{**}(\rho) = \phi_{\beta}(\rho)$ in (ρ', ρ'')

LMP plus hard cores.

Fix:

β in a suitable interval;

the hard core radius R suitably small;

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Put in a cube $\Lambda \subset \mathbb{R}^3$ of large side L a mass $\rho|\Lambda|$ and observe the system by partitioning Λ into cubes $C^{(\ell)}$ of side $\ell \ll L$.

We observe different behaviors when varying ρ .

The gas phase.

For small densities ρ :

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- ▶ This is uniform no matter how large is L
- ▶ Accuracy improves with ℓ : less and less probable to be in the unlikely event, the fraction of bad cubes decreases, in the good cubes closeness to ρ improves.

Phase transition.

The gas phase persists till $\rho \leq \rho_{\beta,\gamma;R}^-$.

In the interval $(\rho_{\beta,\gamma;R}^-, \rho_{\beta,\gamma;R}^+)$ there is a phase transition.

Take $\rho \in (\rho_{\beta,\gamma;R}^-, \rho_{\beta,\gamma;R}^+)$, then

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E. Pulvirenti, D. Tsagkarogiannis and EP, in preparation.

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The pure hard spheres system in $d = 3$ has a phase transition (from disorder to order) with forbidden density interval (ρ', ρ'') (as suggested by numerical computations).

The liquid phase persists till $\rho \leq \rho'$ while the system is in its solid phase when $\rho \geq \rho''$.

For $\rho \in (\rho', \rho'')$ there are microstructures.

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- ▶ Second regime. $\ell > \gamma^a$, $a > 1$, then in a large fraction of cubes $C^{(\ell)}$ the density is close to ρ .
- ▶ The picture is uniform in L . The second regime gets sharper as ℓ increases while to have sharper accuracy in the first regime we must take γ smaller.

Rigorous results.

Microstructures have been found as minimizers of free energy functionals in anelastic crystals and micromagnetism.

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Periodic minimizers in the $d = 1$ case with computation of period. Bounds in $d > 1$.

One dimensional Ising at $T > 0$.

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For $\beta > 1$: $\phi_\beta^{**}(m) < \phi_\beta(m)$ for $|m| < m_\beta$,
 $m_\beta = \tanh\{\beta m_\beta\} > 0$.

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The competition here is between the Kac energy which plays the role of the short range forces while the long range forces are due to the entropy which in $d = 1$ is so strong to prevent phase transitions.

DLR measures

By equivalence of ensembles we can reduce to study the typical configurations of DLR measures with magnetic field h (and $\beta > 1$). Relevant h are those for which the average spin m varies in $(-m_\beta, m_\beta)$.

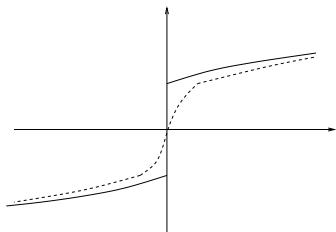


Figure: m versus h in mean field and $\gamma > 0$ (dashed line)

Turns out that: $h \approx e^{-c\gamma^{-1}}$.

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Introduce a phase indicator: $\Theta(x; \sigma)$: $\Theta(x; \sigma) = \pm 1$ means that empirical averages around x are close to $\pm m_\beta$; otherwise $\Theta(x; \sigma) = 0$ no phase can be recognized at x .

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The process $\{\sigma(x), x \in \mathbb{Z}\}$ is Markov with range γ^{-1} (Spitzer).

Too many information in σ , we just want to know where empirical magnetization is close to $\pm m_\beta$.

Introduce a phase indicator: $\Theta(x; \sigma)$: $\Theta(x; \sigma) = \pm 1$ means that empirical averages around x are close to $\pm m_\beta$; otherwise $\Theta(x; \sigma) = 0$ no phase can be recognized at x .

Definition such that intervals with $\Theta = 1$ and $\Theta = -1$ are separated by $\Theta = 0$.

Interfaces

σ gives rise to a sequence (ℓ_i, ℓ'_i) , $i \in \mathbb{Z}$: ℓ_i length of i -th interval with $\Theta \geq 0$; ℓ'_i length of the successive interval with $\Theta \leq 0$.

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However we can cluster together the intervals in a suitable way so that the clustered intervals have the law of a renewal process.