Metastability for continuum interacting particle systems

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Sixth Workshop on Random Dynamical Systems
Bielefeld, 31 October 2013

Problem

Question:
How long does it take to go from *gas* to *condensed* phase? Typically, if the density is only slightly larger than *saturation density*: it takes a long time – there is a nucleation barrier to overcome.
Physics / thermodynamics: topic of nucleation theory.

This talk:
stochastic approaches to metastability for Markovian dynamics whose stationary measures are Gibbs measures. Adapt existing results for lattice spin systems to continuum. Bianchi, Bovier, Eckhoff, den Hollander, Gayrard, Ioffe, Klein, Manzi, Nardi, Spitoni...

Limitations:
We *do not know* whether the system actually has a gas / condensed phase transition at positive temperature. But: this does not bother us because we work in the zero-temperature limit at fixed finite volume.

Moreover, *artificial dynamics* – particles appear and disappear out of the blue. Expected: methods carry over to a whole class of Markovian dynamics.

Outline

1. Model
2. Main result
3. Key proof ingredient: potential-theoretic approach
4. Application to our problem

Grand-canonical Gibbs measure

- $L > 0$, box $\Lambda = [0, L] \times [0, L]$.
- $\beta > 0$ inverse temperature, $\mu \in \mathbb{R}$ chemical potential
- $v : [0, \infty) \to \mathbb{R} \cup \{\infty\}$ pair potential – *soft disk potential* Radin '81

$$v(r) = \begin{cases} \infty, & r < 1 \\ 24r - 25, & 1 \leq r \leq 25/24, \\ 0, & r > 25/24. \end{cases}$$

- Total energy $U(\{x_1, \dots, x_n\}) := \sum_{i<j} v(|x_i - x_j|)$, $U(\emptyset) = U(\{x\}) = 0$.
- Probability space:

$$\Omega := \{\omega \subset \Lambda \mid \mathrm{card}(\omega) < \infty\}.$$

Reference measure: Poisson point process Q, intensity parameter 1.
Grand-canonical Gibbs measure $P = P_{\beta,\mu,\Lambda}$

$$\frac{\mathrm{d}P}{\mathrm{d}Q}(\omega) = \frac{1}{\Xi} \exp\Big(-\beta\big(U(\omega) - \mu n(\omega)\big)\Big),$$

$n(\omega) := \mathrm{card}(\omega) =$ number of points in configuration ω.
$\Xi = \Xi_\Lambda(\beta, \mu)$ grand-canonical partition function.

Dynamics

Combine interaction energy and chemical potential

$$H(\omega) := U(\omega) - \mu n(\omega).$$

Dynamics: Metropolis-type Markov process with generator

$$(Lf)(\omega) := \sum_{x\in\omega} \exp\big(-\beta[H(\omega\backslash x) - H(\omega)]_+\big)\Big(f(\omega\backslash x) - f(\omega)\Big) + \int_\Lambda \exp\big(-\beta[H(\omega\cup x) - H(\omega)]_+\big)\Big(f(\omega\cup x) - f(\omega)\Big)\mathrm{d}x.$$

Birth and death process: particles appear and disappear anywhere in the box.
Rates are exponentially small in β if adding / removing particle increases $H(\omega)$.
Grand-canonical Gibbs measure is reversible.

Analogue of spin-flip dynamics for lattice spin systems: Glauber dynamics.
Used in numerical simulations under the name grand-canonical Monte-Carlo.
Studied in finite and infinite volume Glötzl '81; Bertini, Cancrini, Cesi '02; Kuna, Kondratiev, Röckner ...

Warm-up for more "realistic" dynamics (particles hop / diffuse).

Metastable regime

We are interested in the limit $\beta \to \infty$ at fixed μ, fixed Λ.
The equilibrium measure $P_{\beta,\mu,\Lambda}$ will concentrate on minimizers of $H(\omega) = U(\omega) - \mu n(\omega)$. Observe

$$\min_{\omega} H(\omega) = \min_{k\in\mathbb{N}_0} \min_{n(\omega)=k} \big(U(\omega) - \mu n(\omega)\big) = \min_{k\in\mathbb{N}_0} \big(E_k - k\mu\big).$$

Ground states: Radin '81

$$E_k := \min_{n(\omega)=k} U(\omega) = -3k + \left\lceil \sqrt{12k-3} \right\rceil.$$

Every minimizer of U is a subset of a triangular lattice of spacing 1.

Three cases:

1. $\mu < -3$: $k \mapsto E_k - k\mu$ increasing, minimizer $k = 0$.
   Minimum = empty box.
2. $\mu > -2$: $k \mapsto E_k - k\mu$ decreasing, minimizer: k large.
   Minimum = filled box.
3. $-3 < \mu < -2$: local minimum at $k = 0$, global minimum: k large.
   Empty box = metastable, filled box = stable. Metastable regime.

Question: for $\mu \in (-3, -2)$, how long does it take to go from empty to full?

Critical and protocritical droplets

Write $\mu = -3 + h$.
Assumption $h \in (0,1)$ and $h^{-1} \notin \frac{1}{2}\mathbb{N}$.
Set

$$\ell_c := \left\lfloor \frac{1}{h} \right\rfloor .$$

Proposition The map $k \mapsto E_k - k\mu$ has a unique maximizer k_c,

$$k_c = \begin{cases} (3\ell_c^2 + 3\ell_c + 1) - (\ell_c + 1) + 1, & h \in (\frac{1}{\ell_c + 1/2}, \frac{1}{\ell_c}), \\ (3\ell_c^2 + 3\ell_c + 1) + \ell_c + 1, & h \in (\frac{1}{\ell_c + 1}, \frac{1}{\ell_c + 1/2}). \end{cases}$$

Note: $3\ell_c^2 + 3\ell_c + 1 =$ no. of particles in equilateral hexagon of sidelength ℓ_c.

Proposition Let $k_p := k_c - 1$. The minimizer of $U(\omega)$ with $n(\omega) = k_p$ is unique, up to translations and rotations – obtained from an equilateral hexagon of sidelength ℓ_c by adding or removing one row. Protocritical droplet.
Critical droplet = protocritical droplet + a protuberance.

Proof: builds on Radin '81. Related: Au Yeung, Friesecke, Schmidt '12.

Generalization of known results for Ising / square lattice to triangular lattice + continuum degrees of freedom.

Target theorem

Time to reach dense configurations:

$$D = \{\omega \in \Omega \mid n(\omega) \geq \rho_0 |\Lambda|\},$$
$$\tau_D := \inf\{t > 0 \mid \omega_t \in D\}.$$

$\rho_0 \approx$ density of the triangular lattice.

Goal: as $\beta \to \infty$,

$$\boxed{\mathbb{E}_\emptyset \tau_D = \big(1 + o(1)\big)\, C(\beta)^{-1} \exp(\beta\Gamma)}.$$

Energy barrier:

$$\Gamma = \max_{k \in \mathbb{N}} \big(E_k - k\mu\big) = E_{k_c} - k_c \mu.$$

Prefactor:

$$C(\beta) \approx 2\pi\, |\Lambda| \times \frac{1}{(24\beta)^{2k_c - 3}} \times \text{a finite sum over critical droplet shapes.}$$

Might have to settle for different set $\tilde{D}$ because of the complex energy landscape.

Generalizes results for Glauber dynamics on square lattice. Principal difference: prefactor β-dependent. Appearance of derivative $v'(1+) = 24$ reminiscent of Eyring-Kramers formula (transition times for diffusions). Blends discrete and continuous aspects.

Details & interpretation

Inverse of the hitting time: intermediate expression

$$\left(\mathbb{E}_{\emptyset}\tau_D\right)^{-1} \sim \frac{1}{\Xi} \int_{\{n(\omega)=k_c\}} \frac{|L(\omega)|}{1+|L(\omega)|} \exp\left(-\beta H(\omega)\right) Q(\mathrm{d}\omega).$$

with

$$L(\omega) = \left\{y \in \Lambda \mid H(\omega \cup y) \leq H(\omega) \text{ and } (*)\right\} \subset \Lambda$$

(*) there is a sequence $\omega_k = \omega \cup \{y, y_1, \dots, y_k\}$ $k = 1, \dots, n$ such that $H(\omega_k) < \Gamma$ for all k and $\omega_n \in D$.

Evaluation:

- As $\beta \to \infty$, only a small neighborhood of critical droplets (quasi-hexagon + protuberance) contributes to the integral.
- $|L(\omega)|/(1 + |L(\omega)|)$ = probability that a critical droplet ω grows rather than shrinks.
- probability of seeing a critical droplet: $2\pi|\Lambda|$ (position in space + orientation) $\times$ a Laplace type integral over droplet-internal degrees of freedom.
- Evaluation as $\beta \to \infty$ leads to powers of β, sum over possible shapes of critical droplets (location of the protuberance).

Potential theoretic approach

(X_t) irreducible Markov process with finite state space V, transition rates $q(x,y)$, $(x \neq y)$. Reversible measure $m(x)$. Conductance:

$$c(x,y) = m(x)q(x,y) = m(y)q(y,x).$$

A, B disjoint sets, $A = \{a\}$ singleton. Representation of the hitting time:

$$\boxed{\mathbb{E}_a \tau_B = \frac{1}{\mathrm{cap}(a,B)} \sum_{x \in V} h(x) m(x)}$$

$h(x) = \mathbb{P}_x(\tau_a < \tau_B)$ unique solution of the Dirichlet problem

$$h(a) = 1, \quad h(b) = 0 \quad (b \in B),$$
$$(Lh)(x) = \sum_{y \in V,\ y \neq x} q(x,y)\big(h(y) - h(x)\big) = 0 \ (x \in V \backslash (\{a\} \cup B)).$$

"Capacity" or effective conductance:

$$\mathrm{cap}(a,B) = \sum_{y \in V} q(a,y)\big(h(a) - h(y)\big) = (-Lh)(a).$$

Well-known formulas. Have analogues for continuous state spaces.

Potential theoretic approach, continued

Dirichlet form and Dirichlet principle:

$$\mathcal{E}(f) = \frac{1}{2} \sum_{x,y \in V} c(x,y)\big(f(y) - f(x)\big)^2$$

$$\mathrm{cap}(A,B) = \min\big\{\mathcal{E}(f) \mid f|_A = 1,\ f|_B = 0\big\}.$$

Instead of computing hitting times, we have to estimate capacities. Facilitated by variational principles: Dirichlet, Thomson, Berman-Konsowa.

Remark: vocabulary (capacity / conductance) hybrid of two distinct pictures:

- Random walks $\leftrightarrow$ electric networks: network of resistors, $c(x,y) = 1/r(x,y) =$ conductance, $f(x) =$ voltage at node x, $\mathcal{E}(f) =$ power of dissipated energy. Think

$$\mathcal{P} = UI = RI^2 = CU^2.$$

- Probabilistic potential theory (Brownian motion $\leftrightarrow$ Laplacian): Dirichlet form $=$ electrostatic energy, think

$$\mathcal{E}(\varphi) = \frac{1}{2} \int \varepsilon(x) |\nabla \varphi(x)|^2 \mathrm{d}x.$$

Gaudillière '09: Condenser physics applied to Markov chains: a brief introduction to potential theory. Notes from the XII. Brazilian school of probability.

Application to continuum Glauber dynamics

Dirichlet form:

$$\mathcal{E}(f) = \frac{1}{2}\int_\Omega f(x)\big(-Lf\big)(x) P_{\beta,\mu,\Lambda}(\mathrm{d}\omega)$$
$$= \frac{1}{2}\frac{1}{\Xi}\int_\Omega\int_\Lambda e^{-\beta\max(H(\omega),H(\omega\cup x))}\big(f(\omega\cup x) - f(\omega)\big)^2 \mathrm{d}x\, Q(\mathrm{d}\omega)$$

Network with edges $(\omega, \omega\cup x)$, conductances $\exp(-\beta\max[H(\omega), H(\omega\cup x)])$.
More precisely: conductance is a measure $K(\mathrm{d}\omega, \mathrm{d}\tilde{\omega})$ on $\Omega\times\Omega$,

$$\mathcal{E}(f) = \frac{1}{2}\int_{\Omega\times\Omega}\big(f(\omega) - f(\tilde{\omega})\big)^2 K(\mathrm{d}\omega, \mathrm{d}\tilde{\omega}).$$

Wanted: effective conductance (capacity) between $A = \{\emptyset\}$ and $B = D =$ dense configurations as $\beta\to\infty$.

Upper bound with Dirichlet principle – $\mathrm{cap}(\emptyset, D) \leq \mathcal{E}(f)$, $f =$ guessed good test function.

Lower bound with Berman-Konsowa principle: capacity as a *maximum* over probability measures on paths from $\emptyset$ to D.

Finite state space: Berman, Konsowa '90.

Reversible jump processes in Polish state spaces den Hollander, J. (in preparation).

Berman-Konsowa principle and state of the proof

Berman-Konsowa principle: den Hollander, J. '13

- $\mathbb{P}$ probability measure on paths $\gamma = (\omega_0, \ldots, \omega_n)$ from $\emptyset$ to D
- $\Phi_{\mathbb{P}}$ *flow*: $\Phi_{\mathbb{P}}(C_1 \times C_2)$ = expected no. of edges from C_1 to C_2 (*measure*).
- Variational representation for the capacity:

$$\mathrm{cap}(\emptyset, D) = \sup_{\mathbb{P}} \mathbb{E}\Big[\Big(\sum_{(x,y)\in\gamma} \frac{\mathrm{d}\Phi_{\mathbb{P}}}{\mathrm{d}K}(x,y)\Big)^{-1}\Big].$$

- Lower bound for the capacity: guess a test measure $\mathbb{P}$ on paths.

State of the proof for asymptotics of the hitting time:

- Proof nearly complete for time to become *supercritical*, i.e., modified choice of D

$$\tilde{D} = \{\omega \in \Omega \mid n(\omega) \geq k_c + 1\}.$$

- For original choice $D = \{n(\omega) \geq \rho_0 |\Lambda|\}$, need to answer an additional question about energy landscape, "no-deep-well property". **Open**.

If property does not hold, it is possible that the Glauber dynamics gets stuck in configuration in $\tilde{D} \backslash D$.