Metastability for continuum particle systems

R. Kotecký

A joint work with F. den Hollander (Leiden), S. Jansen (Bochum) and E. Pulvirenti (Leiden)

Warwick/Prague

Models in continuum

- Phase transitions for particle systems on continuum :
  To find a rigorous justification of a liquid-gas phase transition for a realistic particle systems on continuum (say, with the Lenard-Jones interaction) is still an open problem. Rigorous proof of the presence of phase transitions has been achieved only for few models. The main examples are:
  - The Widom-Rowlinson model with a proof of phase transition presented by D. Ruelle , '71.
  - Kac models with 2-body attraction and 4-body repulsion by J. Lebowitz, A. Mazel, and E. Presutti , '99.

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Metastability

Several important steps:

- Nonanalaticity :
  Proof that it is not possible to view metastability in terms of analytic continuation of the phase transition—essential singularity at the transition point proven for Ising model by S. N. Isakov '84 with the help of his own version of the Pirogov-Sinai theory .

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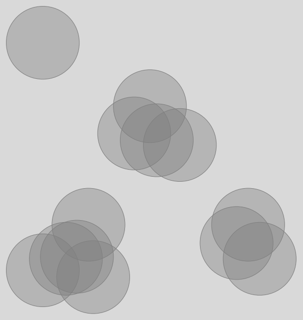
Metastability for Widom-Rowlinson model

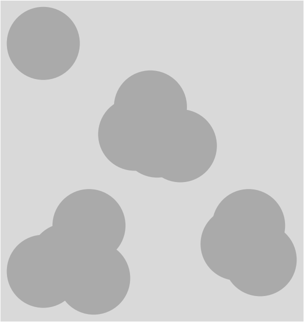
A joint work with F. den Hollander (Leiden), S. Jansen (Bochum) and E. Pulvirenti (Leiden)

Widom-Rowlinson model



Particles in continuum: at positions $\omega = (x_1, x_2, \ldots, x_N)$ interacting with many-body interaction.

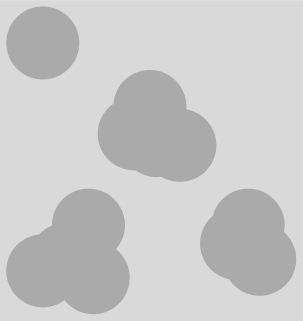
Widom-Rowlinson model



Interaction: $U(\omega) = (W(\omega) - NV_0)\frac{\varepsilon}{V_0}$
Here, W is a union of disks of radius 2 (with V_0 denoting the area of one such disk) and ε is a microscopic energy unit.
U is a many-body attractive stable potential with repulsion replaced by saturation:

$$0 \geq U(\omega) \geq -(N-1)\varepsilon$$

Widom-Rowlinson model

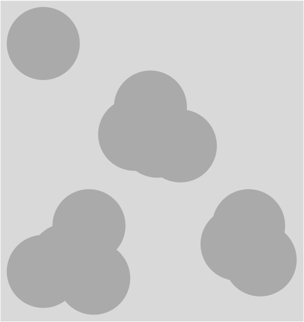


Pressure-temperature ratio Π (in units ε/k):

$$\exp\{\Pi\frac{V}{V_0}\} = \sum_N \frac{\left(\frac{ze^\theta}{V_0}\right)^N}{N!}\int \exp\{-\theta W(\omega)\}d\omega$$

$\theta = \beta/\epsilon$ is the dimensionless temperature and z is the dimensionless activity normalised so that $\rho = \frac{NV_0}{V} \sim z$ in the ideal gas limit.

Hidden symmetry - two colour particle system



Consider two types of particles of radius 1

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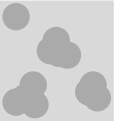
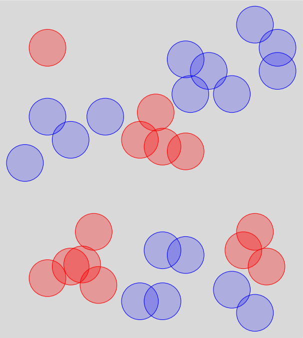
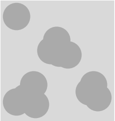
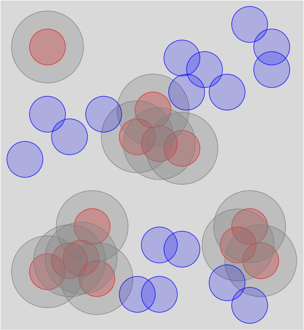




with the hard-core interaction between different species.

Hidden symmetry - two colour particle system





The centres of blue particles must keep off the area $W(\omega_R)$ determined by the red particles.
Integrating out blue particles we get exactly the previous when identifying $z_R = ze^{\theta}$ and $z_B = \theta$:

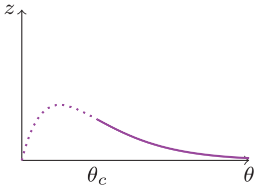
$$\exp\{\Pi_{\mathrm{mix}}\frac{V}{V_0}\} = \sum_{N_R,N_B} \frac{\left(\frac{z_R}{V_0}\right)^{N_R}}{N_R!}\frac{\left(\frac{z_B}{V_0}\right)^{N_B}}{N_B!}\int \mathbb{1}_{\text{Red-Blue hard core}}(\omega_R,\omega_B)d\omega_R d\omega_B =$$

$$= \sum_{N_R} \frac{\left(\frac{z_R}{V_0}\right)^{N_R}}{N_R!}\int \exp\{(V - W(\omega_R))z_B/V_0\}d\omega_R$$

Phase transition

$$\Pi(z,\theta) = -\theta + \Pi_{\mathrm{mix}}(ze^{\theta},\theta)$$

Coexistence line: $z_R = z_B \implies z_t(\theta) = \theta e^{-\theta}$



$\theta > \theta_c$ coexistence of two phases "gas & liquid" for $z = z_t(\theta)$:
Indeed, D. Ruelle '71 (a version of Peierls argument), J. Chayes, L. Chayes, R.K. '95 (stochastic domination by a percolation).

Dynamical WR model

From now on we look back at the original 1-species model.

Heat bath dynamics :
Particle configuration is a continuous-time Markov process $(\omega_t)_{t\geq 0}$ on the state space $\Omega = \cup \Omega_N$ and with generator:

$$(Lf)(\omega) = \int_\Lambda dx\; b(x,\omega)\,[f(\omega \cup x) - f(\omega)] + \sum_{x\in\omega} d(x,\omega)\,[f(\omega \backslash x) - f(\omega)]$$

where particles are added at rate b and removed at rate d:

$$b(x,\omega) = z\, e^{-\theta[U(\omega\cup x) - U(\omega)]}, \quad x \notin \omega, \qquad d(x,\omega) = 1, \quad x \in \omega.$$

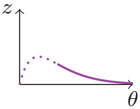
The grand-canonical Gibbs measure is reversible:

$$b(x,\omega)\, e^{-\theta U(\omega)} = d(x, \omega \cup x)\, e^{-\theta U(\omega\cup x)}, \qquad x \notin \omega, \quad \omega \in \Omega.$$

Metastability for the WR model

The aim is to understand the metastable behaviour of $(\omega_t)_{t\geq 0}$, in the following regime:

- fixed volume (torus) Λ and $\theta \to \infty$,



- $z = \kappa\, z_t(\theta)$ with $\kappa \in (1, \infty)$: parameters with stable liquid phase

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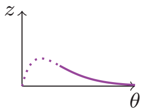
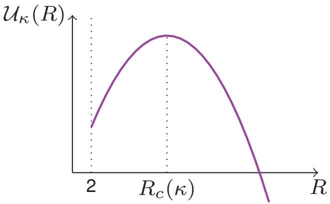


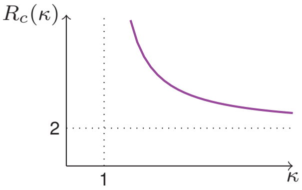
Start with **empty box** $\square = \varnothing$ (supersaturated gas) and wait for the first time the system reaches the **full box** $\blacksquare = \{\omega \in \Omega : W(\omega) = \Lambda\}$.
Questions:

- What is the mean metastable crossover time from $\square$ to $\blacksquare$, i.e. $\tau_{\blacksquare} = \inf\{t > 0\colon\ \omega_t = \blacksquare\}$? Same scaling as the classical Arrhenius law?
- What does the critical droplet look like?

Results

$$R \in [2, \infty) \qquad \mathcal{U}_\kappa(R) = \pi R^2 - \kappa\pi(R-2)^2 \qquad \text{and} \qquad R_c(\kappa) = \frac{2\kappa}{\kappa - 1}.$$





Theorem (1) [dHJKP]: For every $\kappa \in (1, \infty)$,

$$E_\square(\tau_\blacksquare) = \exp\Big[\theta\,\mathcal{U}_\kappa\big(R_c(\kappa)\big) - \theta^{1/3}\,\mathcal{S}_\kappa\big(R_c(\kappa)\big)\,[1 + o_\theta(1)]\Big], \qquad \theta \to \infty.$$

with

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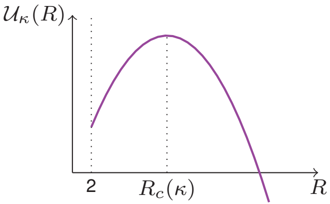

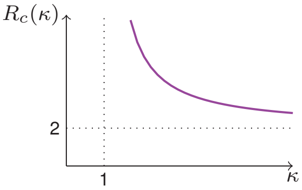

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Theorem (2) [dHJKP]: For every $\kappa \in (1, \infty)$,

$$\lim_{\theta\to\infty} P_\square\big(\tau_\blacksquare / E_\square(\tau_\blacksquare) > t\big) = e^{-t} \qquad \forall\, t \geq 0.$$

Results

Theorem (3) [dHJKP]: For every $\kappa \in (1, \infty)$,

$$\lim_{\theta \to \infty} P_{\square}\left(\tau_{\mathcal{C}_\delta(\kappa)} < \tau_{\blacksquare} \mid \tau_{\square} > \tau_{\blacksquare}\right) = 1$$

where

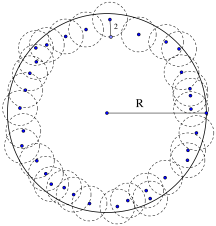
$$\mathcal{C}_\delta(\kappa) = \left\{\omega \in \Omega \colon\ B_{R_c(\kappa)-\delta}(x) \subset W(\omega) \subset B_{R_c(\kappa)+\delta}(x),\ x \in \Lambda\right\}$$

and $\delta(\theta)$ is such that

$$\lim_{\theta \to \infty} \delta(\theta) = 0 \text{ and } \lim_{\theta \to \infty} \theta^{2/3}\delta(\theta) = \infty.$$

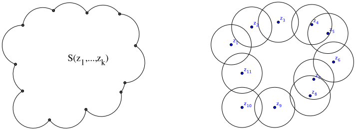
The reason for the entropical term $\theta^{1/3}\,\mathcal{S}_\kappa\big(R_c(\kappa)\big)$

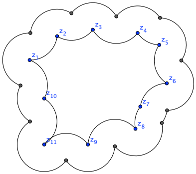
It reflects the bumpiness of the boundary of a droplet.



Integrating over halo shapes?

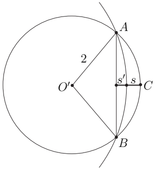
$$\int_\Omega \mathbb{Q}(d\omega)(\kappa\theta)^{N(\omega)}e^{-\theta W(\omega)}\mathbf{1}_{\{W(z)-\pi R^2\in\theta^{-2/3}[0,\delta]\}}$$



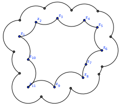


Heuristics for $\theta^{1/3}$

Sticking out by s, the excess area of the halo $\Delta = W(\omega \cup x) - W(\omega)$ is of the order $s^{3/2}$ (and the distance of points A and B about $s^{1/2}$ (to give $ss^{1/2} = s^{3/2}$).



For $e^{-\theta\Delta}$ not to be negligible, it should be $\Delta \sim \theta^{-1}$, yielding for the distance of the centres of boundary circles $s^{1/2} \sim \theta^{-1/3}$ and for the number of boundary circles $n \sim \theta^{1/3}$.



Integrate over $\theta^{1/3}$ positions of centres $z_1, z_2, \ldots$ and determine the behaviour of corresponding integrals in terms of large deviations with the rate $\theta^{1/3}$ and with rate function $\mathcal{S}_\kappa$.