Diffusion d'une particule marquée dans un gaz dilué de sphères dures

Thierry Bodineau

Isabelle Gallagher, Laure Saint-Raymond

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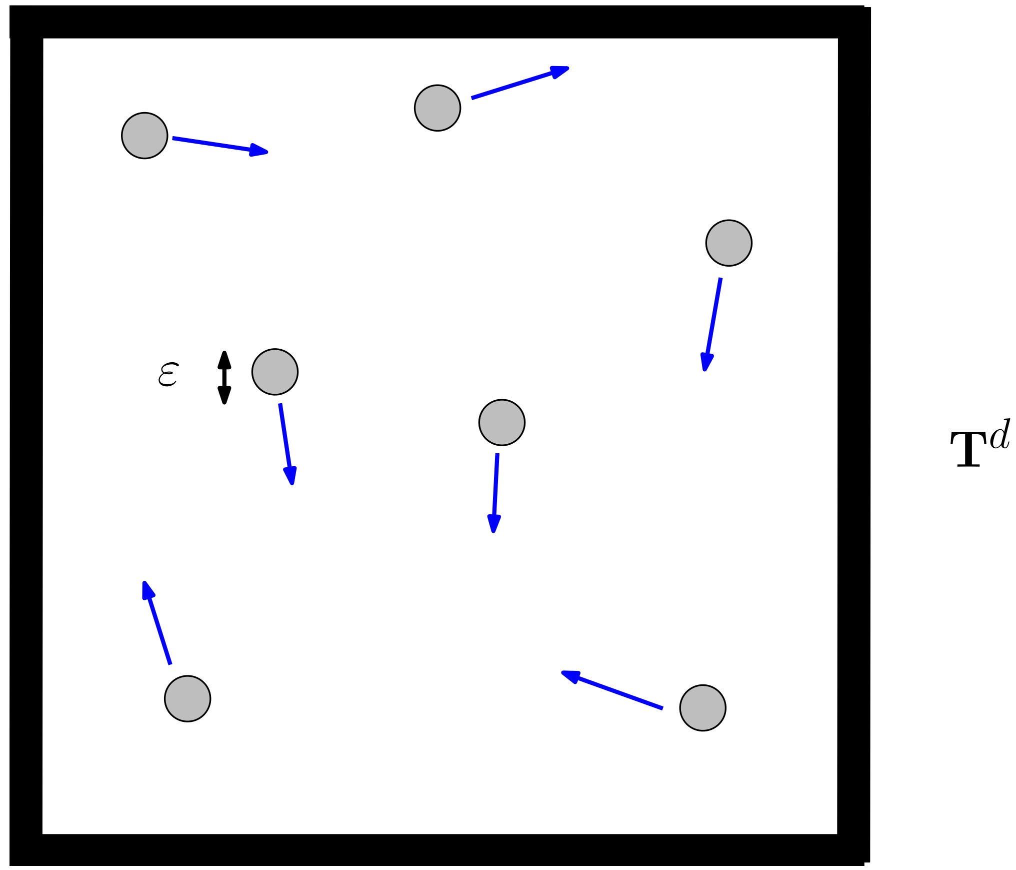
Outline.

- Particle Diffusion
- Introduction

Diluted Gas of hard spheres



Gas of N hard spheres with deterministic Newtonian dynamics (elastic collisions).

Dimension : $d \geq 2$

Periodic domain: $\mathbf{T}^d = [0,1]^d$

Sphere radius = ε

Boltzmann-Grad scaling

$$N\varepsilon^{d-1} = \alpha$$

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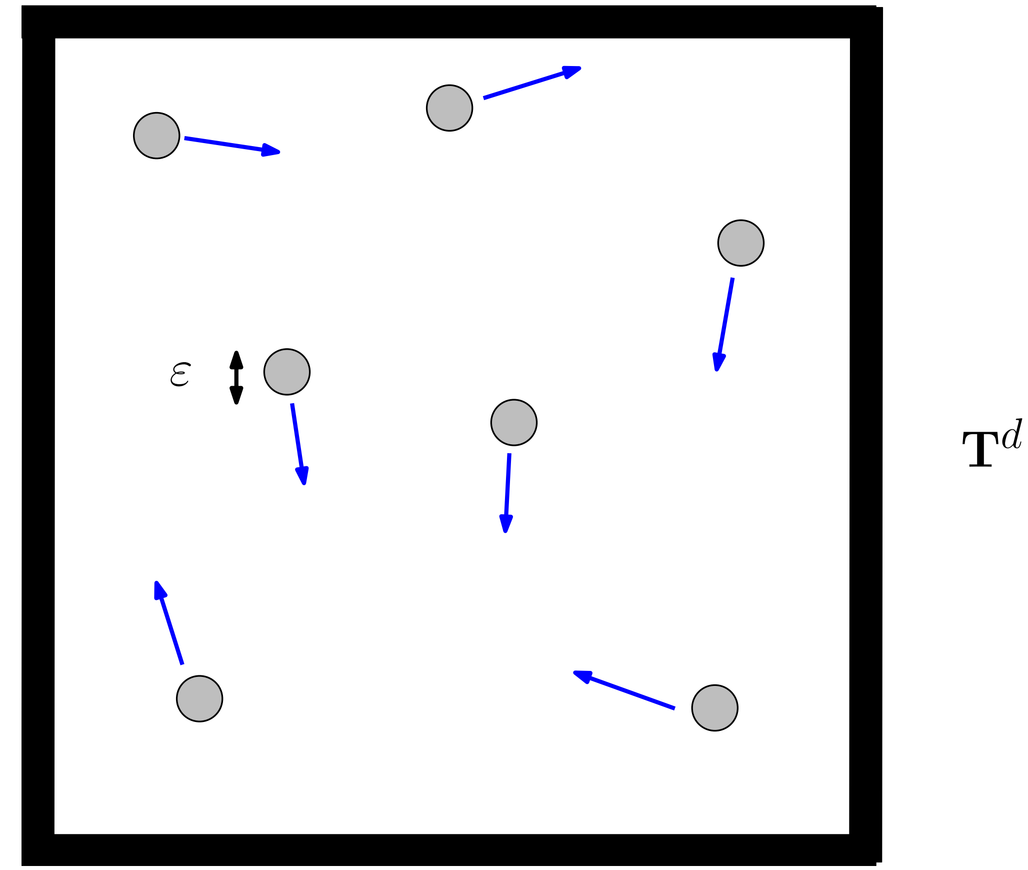
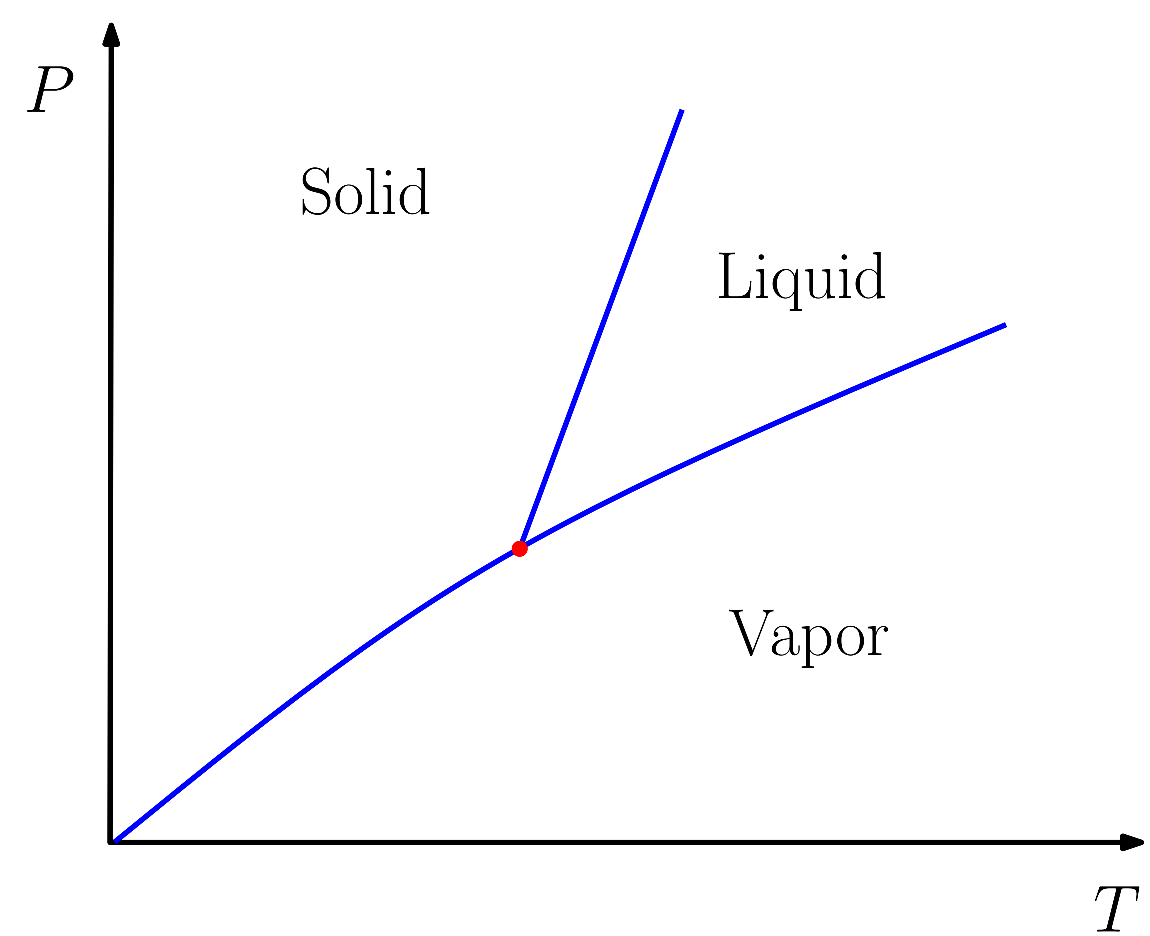
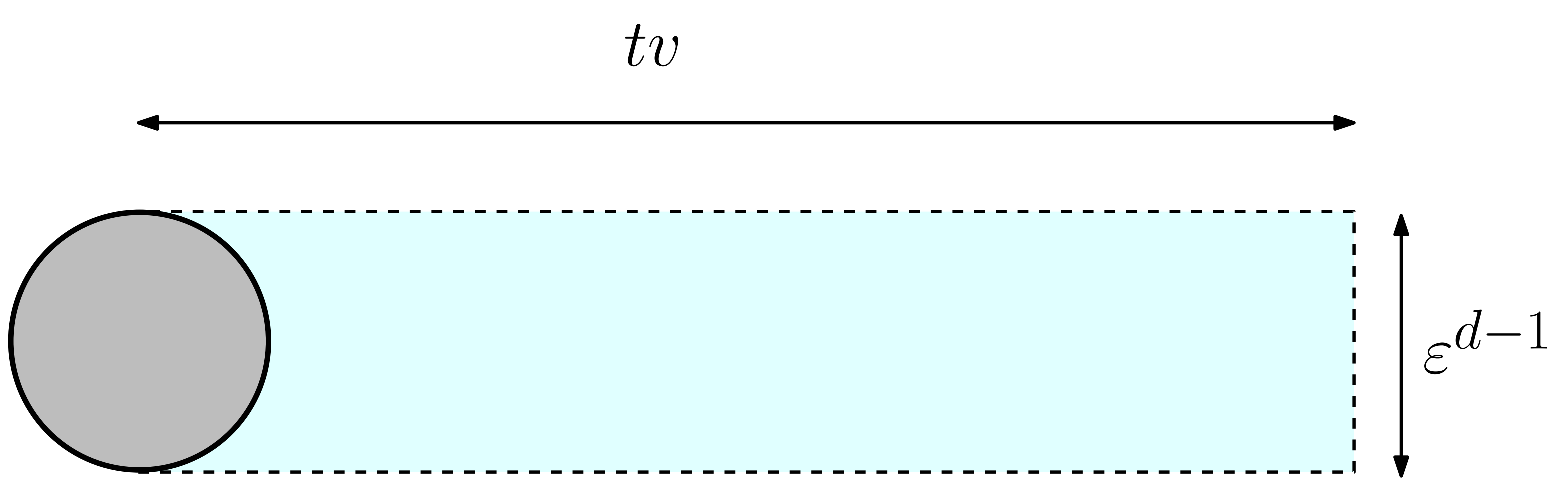




Boltzmann-Grad scaling



- Volume covered by a particle $= tv\varepsilon^{d-1}$
- On average N particles per unit volume

On average, a particle has α collisions per unit of time

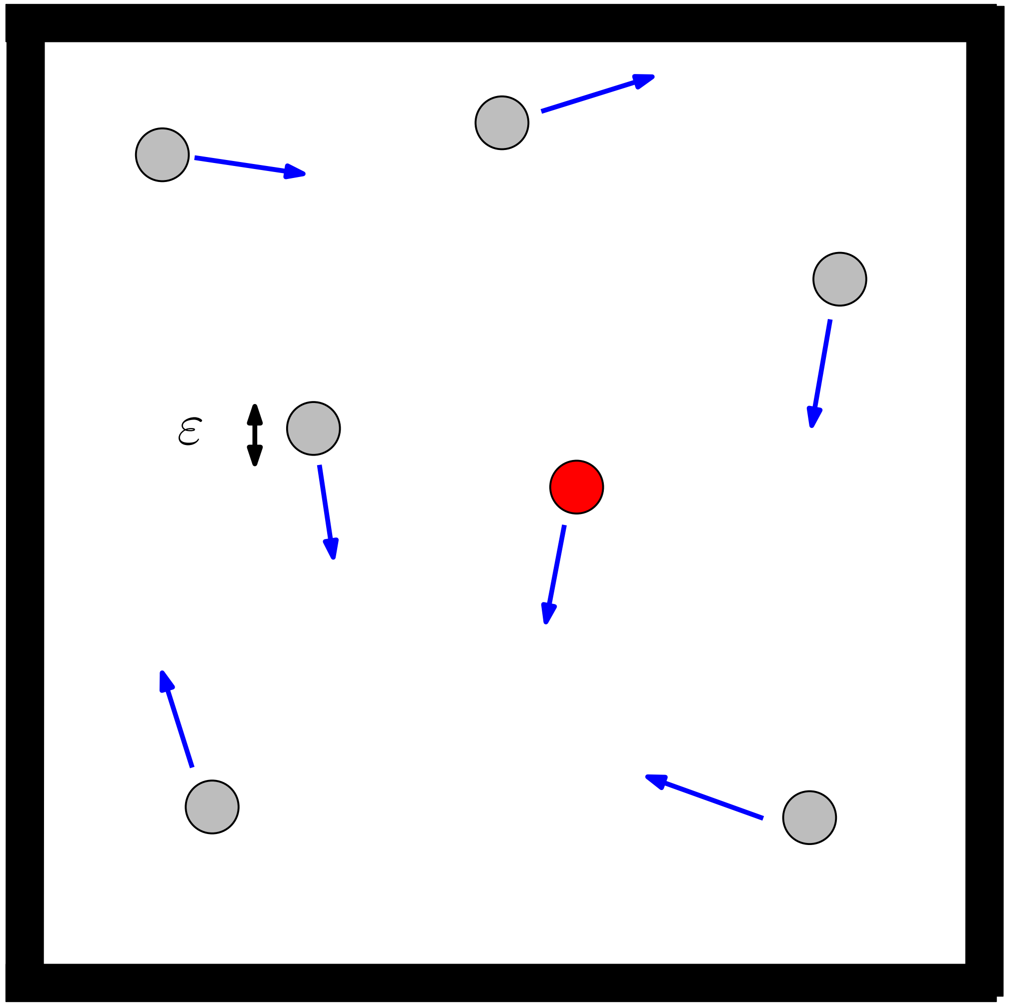
$$N \times \varepsilon^{d-1} \equiv \alpha$$

Diluted Gas of hard spheres

Gas of N hard spheres with deterministic Newtonian dynamics (elastic collisions).

Initial data at equilibrium and a tagged particle (x_1, v_1)

Questions.



In the Boltzmann-Grad scaling

$$N \times \varepsilon^{d-1} \equiv \alpha \text{ and } N \to \infty$$

1. Distribution of $(x_1(t), v_1(t))$

2. Position of the tagged particle $x_1(\alpha t)$ when $\alpha \to \infty$

Hard Sphere dynamics

Gas of N hard spheres : $Z_N = \{(x_i(t), v_i(t)\}_{i\leq N}$

$$\frac{dx_i}{dt} = v_i, \quad \frac{dv_i}{dt} = 0 \quad \text{as long as } |x_i(t) - x_j(t)| > \varepsilon\,,$$

and elastic collisions if $|x_i(t) - x_j(t)| = \varepsilon$

$$\begin{cases} v_i(t^+) = v_i(t^-) - \frac{1}{\varepsilon^2}(v_i - v_j)\cdot(x_i - x_j)(x_i - x_j)(t^-) \\ v_j(t^+) = v_j(t^-) + \frac{1}{\varepsilon^2}(v_i - v_j)\cdot(x_i - x_j)(x_i - x_j)(t^-) \end{cases}$$

Liouville equation for the particle density $f_N(t, Z_N)$

$$\partial_t f_N + \sum_{i=1}^N v_i \cdot \nabla_{x_i} f_N = 0$$

in the phase space

$$\mathcal{D}_\varepsilon^N := \left\{Z_N \in \mathbf{T}_\lambda^{dN} \times \mathbb{R}^{dN} \,/\, \forall i \neq j\,, \quad |x_i - x_j| > \varepsilon\right\}$$

with specular reflection on the boundary $\partial\,\mathcal{D}_\varepsilon^N$.

The tagged particle

Equilibrium distribution

$$M_{N,\beta}(Z_N) = \frac{1}{\mathcal{Z}_{N,\beta}} \exp\Big(-\frac{\beta}{2}\sum_{i=1}^{N}|v_i|^2\Big) \prod_{i\neq j} 1_{|x_i-x_j|>\varepsilon}$$

Particle $Z_1 = (x_1, v_1)$ is tagged. Initial distribution :

$$f_N^0(Z_N) = M_{N,\beta}(Z_N)\,\rho^0(x_1)$$

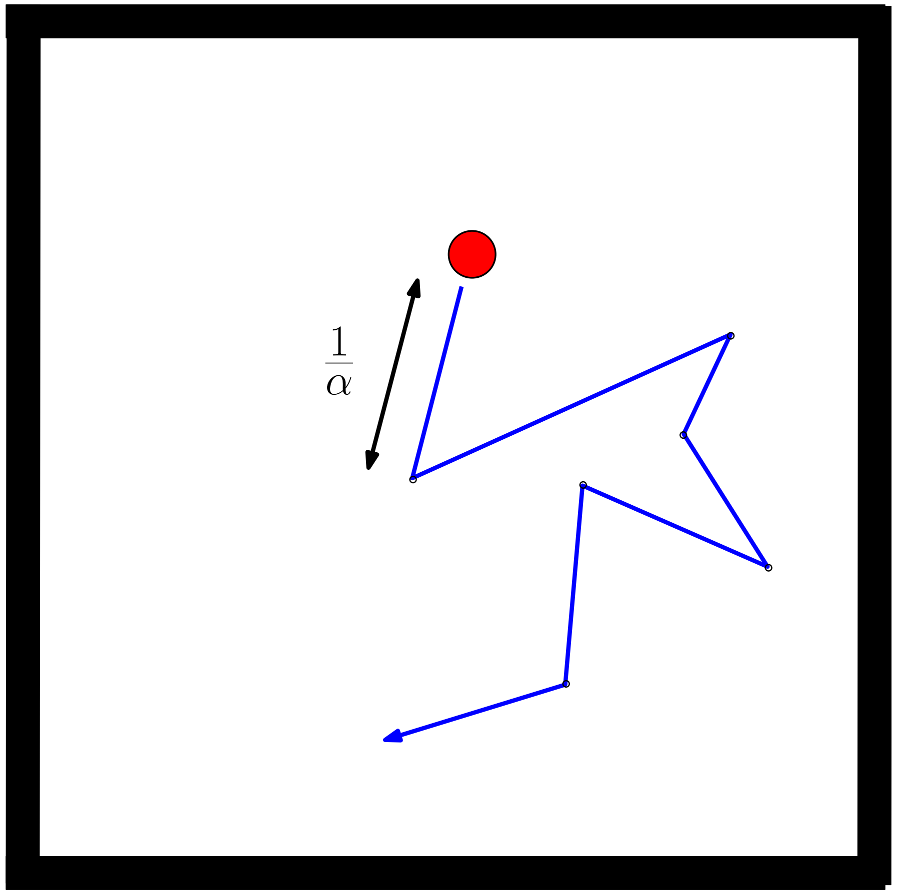
Uniform bound: $\rho^0(x_1) \leq \mu$

Notation: Marginals

$t \geq 0, \forall s \geq 1,$ $$f_N^{(s)}(t, Z_s) = \iint f_N(t, Z_N)\, dz_{s+1} \dots dz_N$$

Tagged particle distribution $f_N^{(1)}(t, (x_1, v_1))$

Limiting stochastic process



single particle dynamics

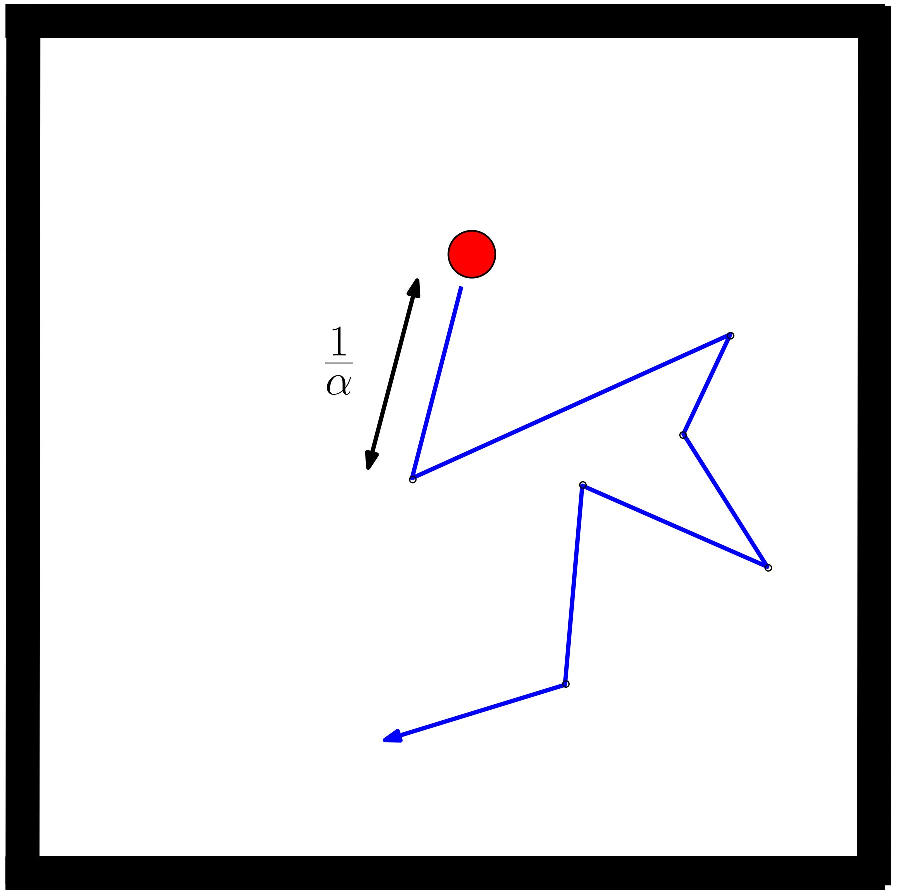
Position : $x(t) = \int_0^t v(u)du$

Markov process on the velocities $\{v(t)\}_{t \geq 0}$ with generator αL

$$Lg(v) := \iint [g(v) - g(v')] \big((v - v_1) \cdot \nu\big)_+ M_\beta(v_1)\, dv_1 d\nu$$

$$v' = v + (\nu \cdot (v_1 - v))\, \nu, \quad v_1' = v_1 - (\nu \cdot (v_1 - v))\, \nu$$

Limiting stochastic process



single particle dynamics

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Markov process on the velocities

$\{v(t)\}_{t\geq 0}$ with generator αL

Particle distribution $M_\beta(v)\varphi_\alpha(x,v,t)$ follows the

Linear Boltzmann equation $\partial_t \varphi + v \cdot \nabla_x \varphi = -\alpha L \varphi$

Probabilist approaches :

Tanaka, Sznitman, Méléard, Graham, Fournier ...

[van Beijeren, Lanford, Lebowitz, Spohn]

N particle system

$f_N^{(1)}(x_1, v_1, t)$

$\alpha = N\varepsilon^{d-1}$

$N \to \infty$

$t > 0$

Linear Boltzmann equation

$\varphi_\alpha(x_1, v_1, t)\, M_\beta(v_1)$

[van Beijeren, Lanford, Lebowitz, Spohn]

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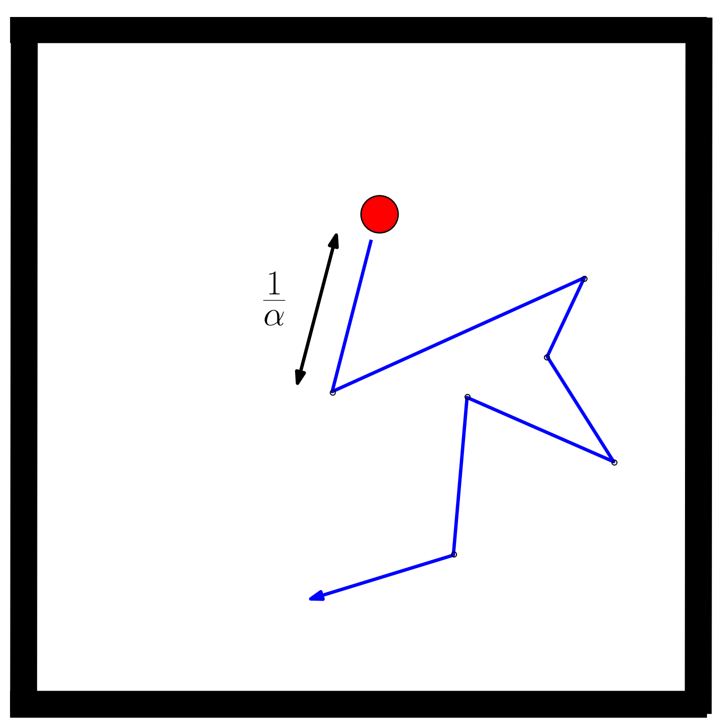
$t = \alpha\,\tau$

$\alpha \to \infty$

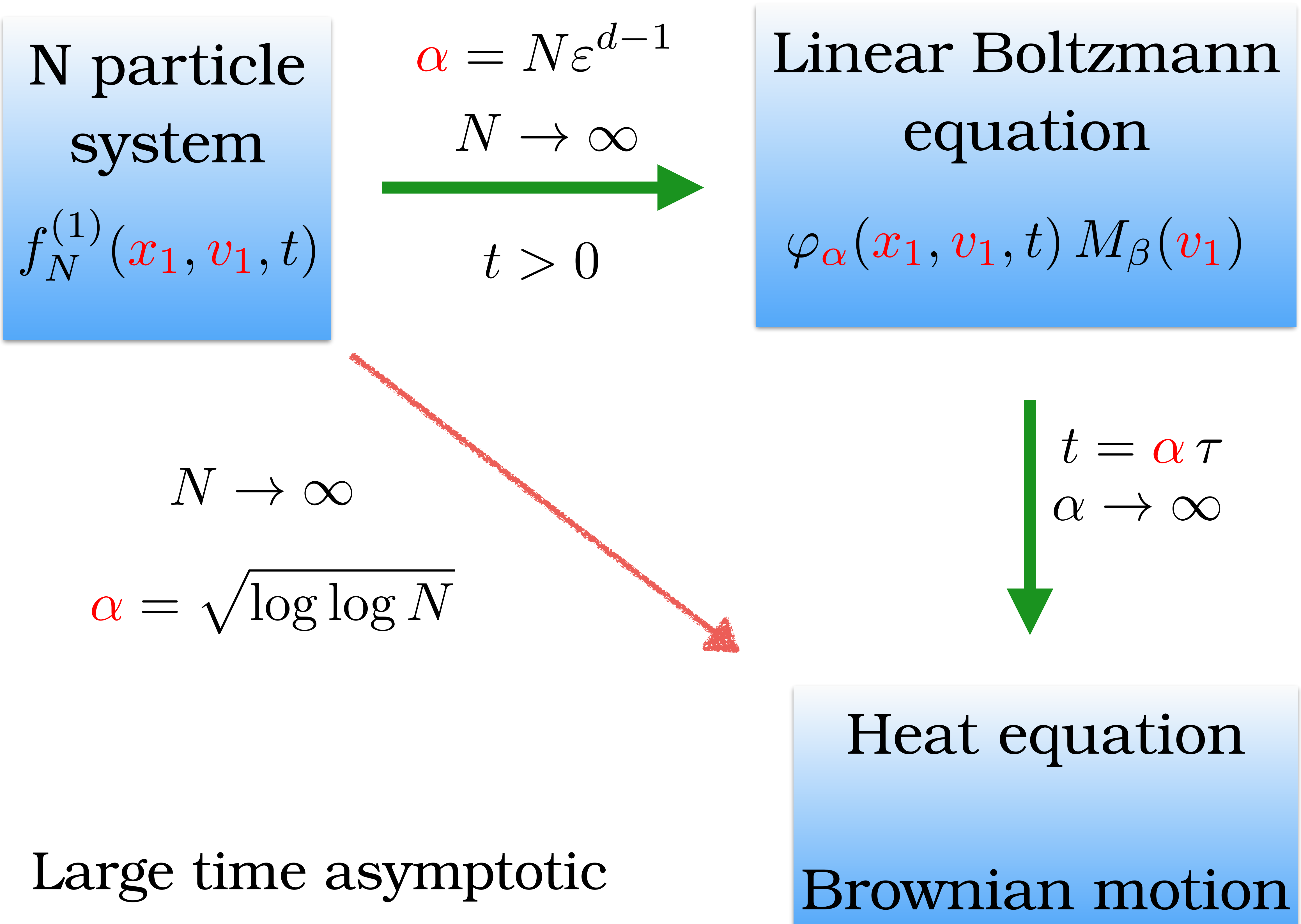


Large time asymptotic

Heat equation

Brownian motion

[van Beijeren, Lanford, Lebowitz, Spohn]



Convergence to the Brownian motion

Rescaled position of the tagged particle

$$\chi(\tau) = x_1(\alpha\tau) \quad \text{with} \quad \alpha = \sqrt{\log\log N}$$

Initial data $\quad f_N^0(Z_N) = M_{N,\beta}(Z_N)\, \rho^0(x_1)$

Theorem [B.,Gallagher, Saint-Raymond]

χ converges weakly to a brownian motion with variance κ_β

The distribution of the tagged particle $f_N^{(1)}(x_1, v_1, \alpha\tau)$ converges as $N \to \infty$ to $M_\beta(v_1)\, \rho(x_1, \tau)$

$$\partial_\tau \rho = \kappa_\beta \Delta_x \rho \quad \text{on } \mathbb{R}^+ \times [0,1]^d, \qquad \rho_{|\,\tau=0} = \rho^0$$

Quantum brownian motion: [Erdös, Salmhofer, Yau]

Lorentz gas

Boltzmann equation

Theorem.

For chaotic initial data $f_N^0(Z_N) \simeq \prod_{i=1}^N f^0(z_i)$ the density of the particle system converges up to a time t >0 to the solution of the Boltzmann equation when $N \to \infty,\ N\varepsilon^{d-1} = \alpha$

$$\partial_t f + v \cdot \nabla_x f$$
$$= \iint_{\mathbf{S}^{d-1}\times\mathbb{R}^d} [f(v')f(v_1') - f(v)f(v_1)] \big((v - v_1)\cdot\nu\big)_+ dv_1 d\nu$$

with $v' = v + \nu\cdot(v_1 - v)\,\nu\,, \quad v_1' = v_1 - \nu\cdot(v_1 - v)\,\nu$

[Lanford], [King], [Alexander], [Uchiyama], [Cercignani, Illner, Pulvirenti], [Simonella], *[Gallagher, Saint-Raymond, Texier]*, [Pulvirenti, Saffirio, Simonella]

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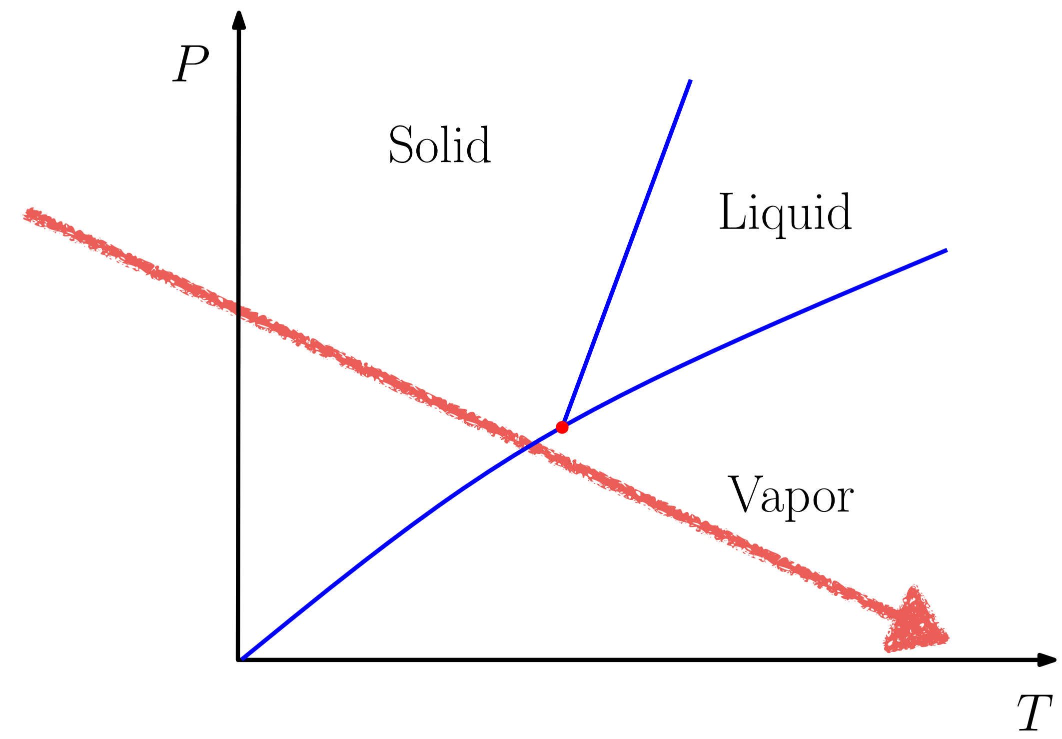
$$\partial_t f + v \cdot \nabla_x f = \iint_{\mathbf{S}^{d-1} \times \mathbb{R}^d} [f(v')f(v'_1) - f(v)f(v_1)] \big((v - v_1) \cdot \nu\big)_+ dv_1 d\nu$$

with $v' = v + \nu \cdot (v_1 - v)\,\nu\,, \quad v'_1 = v_1 - \nu \cdot (v_1 - v)\,\nu$

Lanford's strategy leads to a short time convergence which depends on f^0. The convergence time remains short even if initially the system starts from equilibrium !!!

Equilibrium Properties

- Boltzmann-Grad : $N \times \varepsilon^{d-1} \equiv \alpha$
- Low density : $N \times \varepsilon^{d} = \rho \ll 1$
- High density : $N \times \varepsilon^{d} = \rho \gg 1$



Open Problem : Vapor/Solid phase transition.

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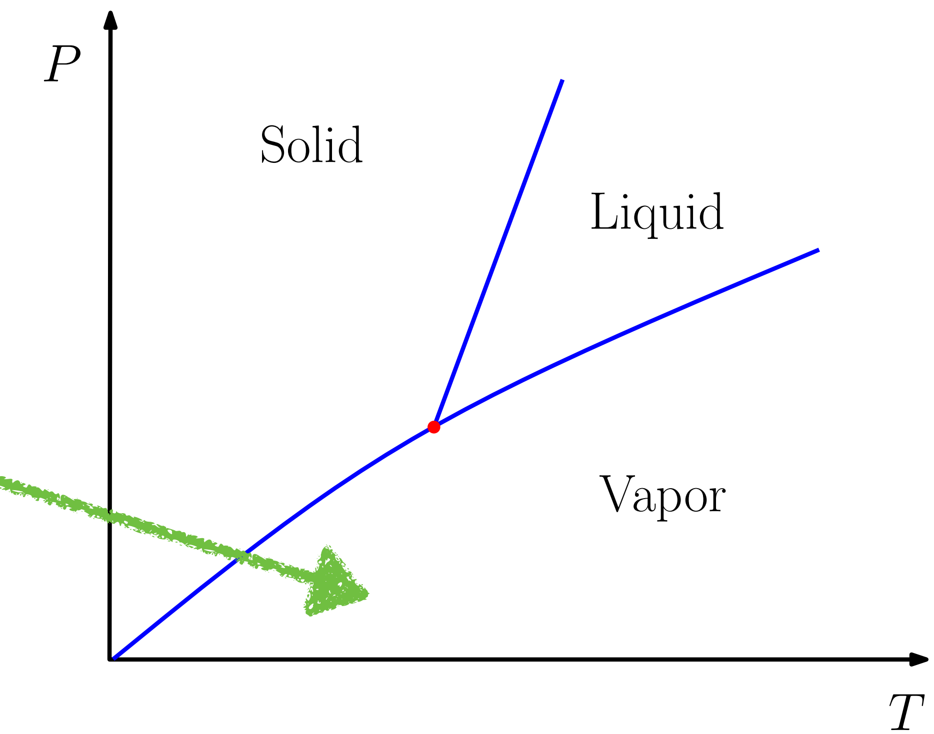

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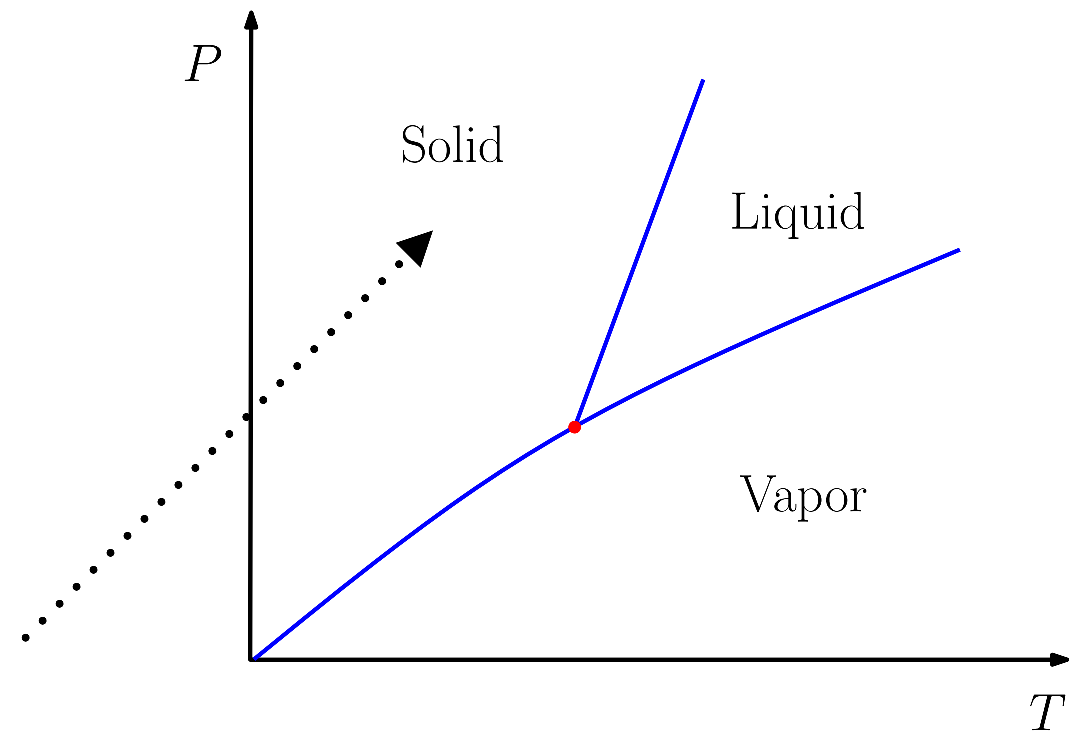

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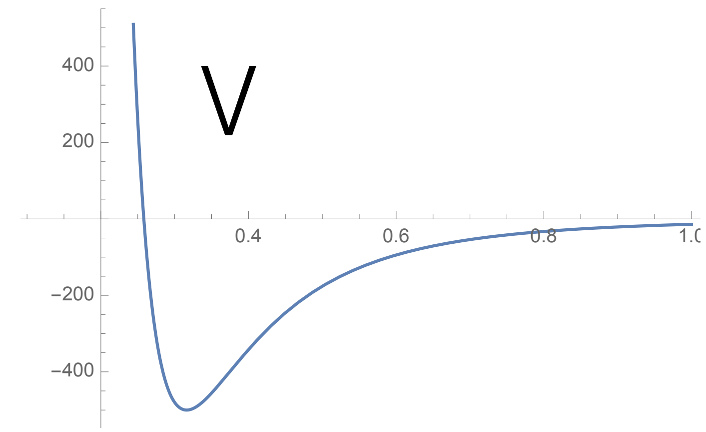
Liquid/Vapor phase transition

Interaction potential

Lennard-Jones potential



$$H(X) = -\sum_{i,j} V\left(\frac{x_i - x_j}{\varepsilon}\right)$$

Gibbs measure $X = \{x_i \in [0,1]^d;\ i \leq N\}$

$$\mu_{N,T}(X) = \frac{1}{Z_{N,T}} \exp\left(-\frac{1}{T} H(X)\right)$$

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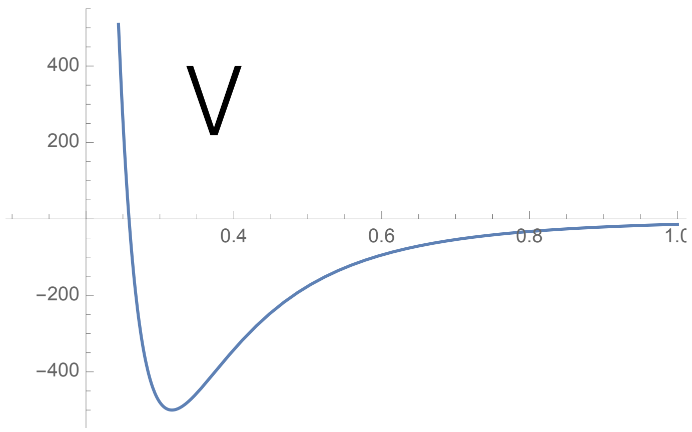

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There is a density $\rho = N\varepsilon^d$ and a temperature T

$$\mu_{N,T}\Big(\text{Phase transition}\Big) \xrightarrow{N\to\infty} 1$$

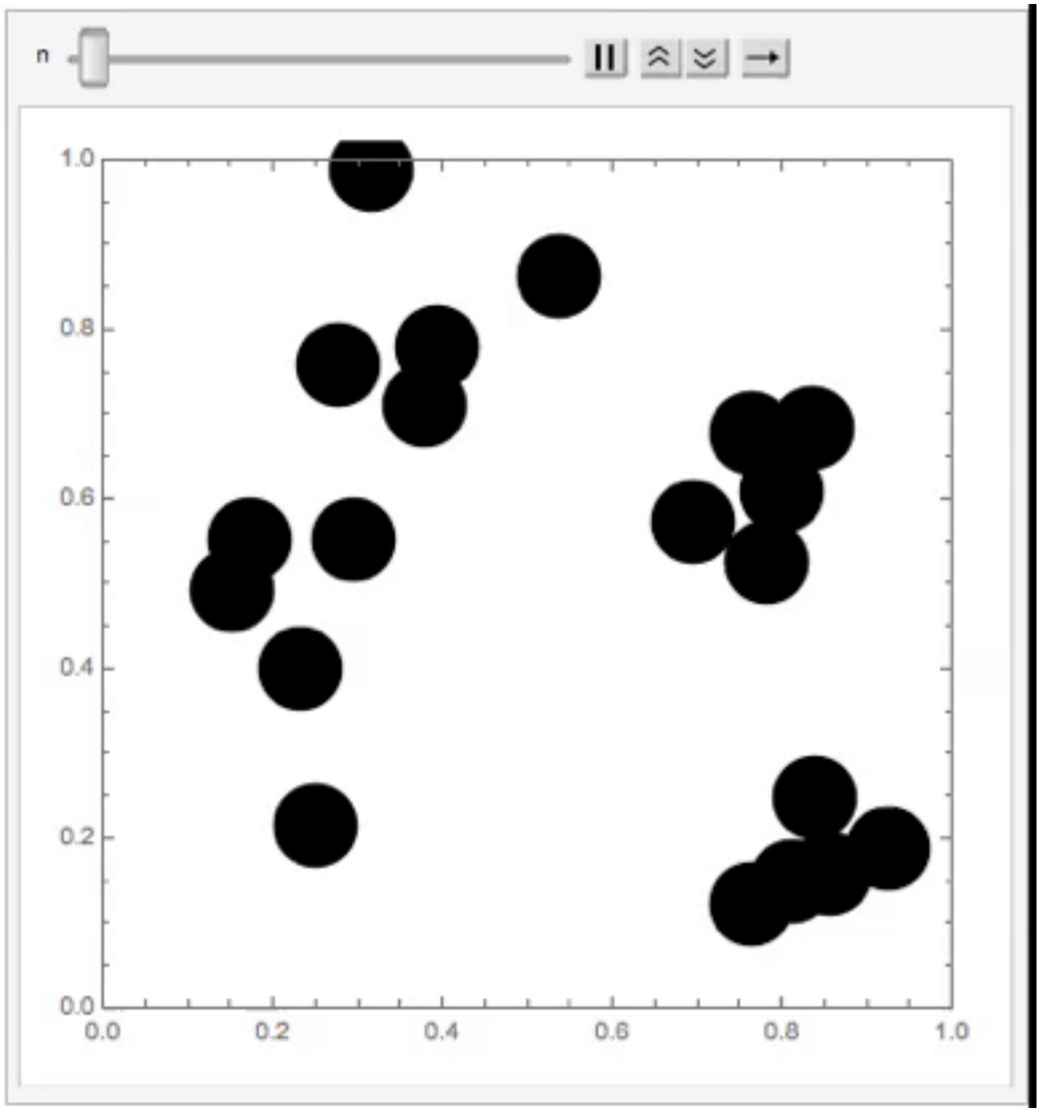
[Lebowitz,Mazel, Presutti]

Continuum percolation

Disks of radius ε randomly distributed

No interaction, No exclusion.

density $\rho = N\varepsilon^d$



Phase transition : $N \to \infty$

- $\rho < \rho_c$: small percolation clusters
- $\rho > \rho_c$: percolation of a macroscopic cluster

Many more models : R. Marchand

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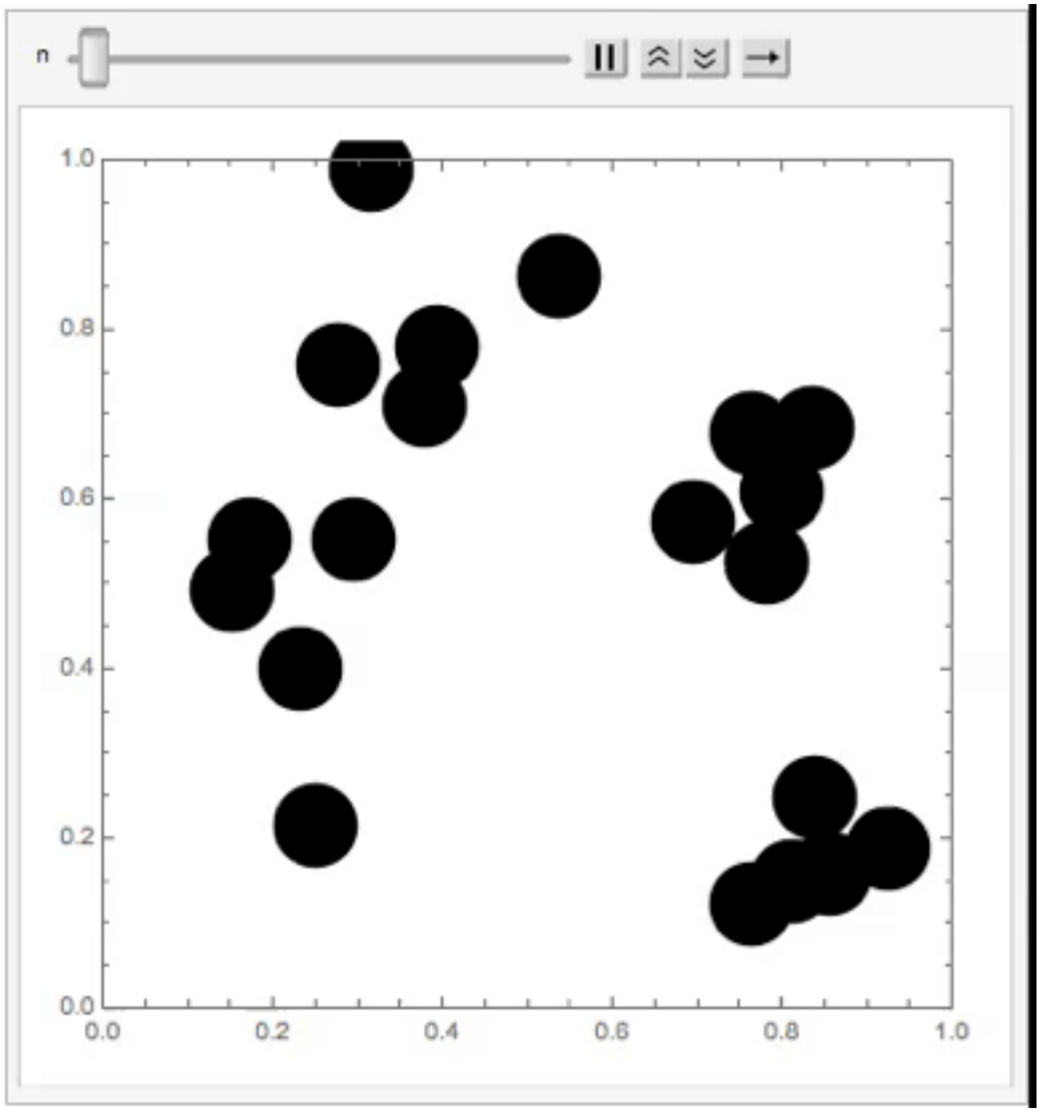


Many more models : R. Marchand

Lattice gas models

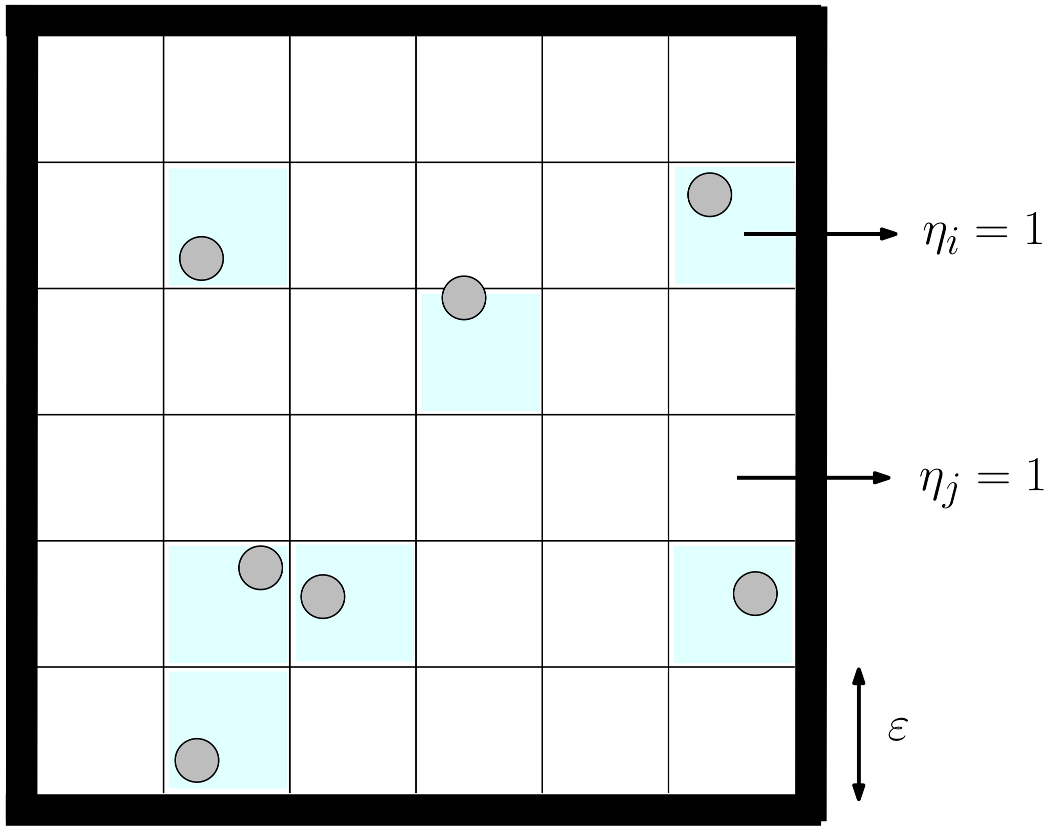
Simplifying the model:

- discrete variables

  $$\eta_i \in \{0,1\} \text{ with } i \in \{1,\dots,\tfrac{1}{\varepsilon}\}^d$$

- nearest neighbor interaction

  $$H(\eta) = -\sum_{i\sim j} \eta_i \eta_j - h \sum_i \eta_i$$



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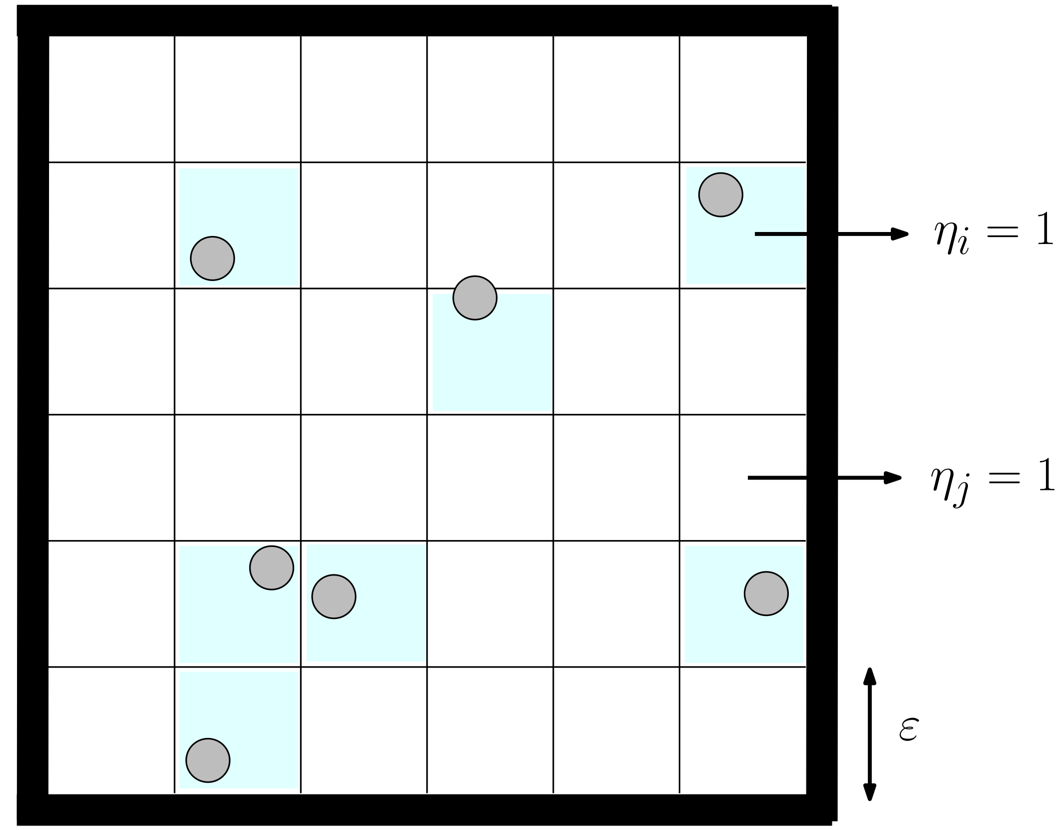

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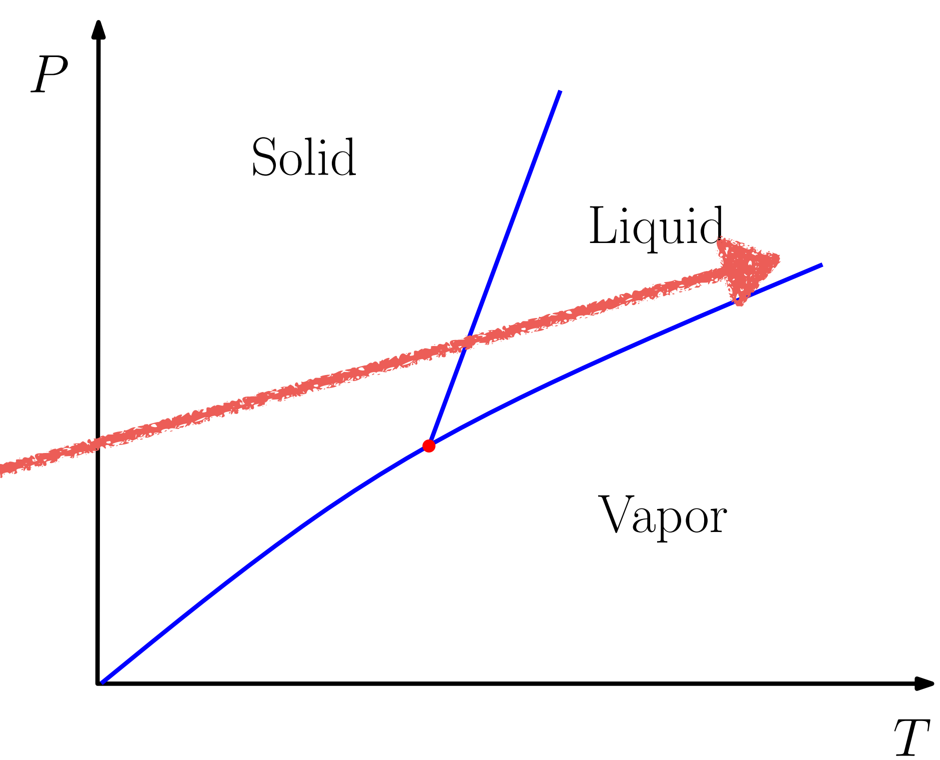

Ising Model : $\sigma_i = 2\eta_i - 1$

B. de Tilière

- **Equilibrium systems** : Gibbs measure

Parameters : (T, h); (T, P)

Critical curve : $T = F\left(h\right)$

- **Non-equilibrium systems** : Local dynamical rules

  - Sandpile models; Driven particle systems …
  - Long range correlations; Self-organized criticality (in general no obvious Hamiltonian)

M. Gorny : A mean field approach