

Polymer Measures and Branching Diffusions

Leonid Koralov

- M. Cranston, L. Koralov, S. Molchanov, B. Vainberg, “Continuous Model for Homopolymers”, JFA (2009).
- L. Koralov, “Branching Diffusion Processes” .

Assume: $v \geq 0$, $\text{supp}(v)$ - compact.

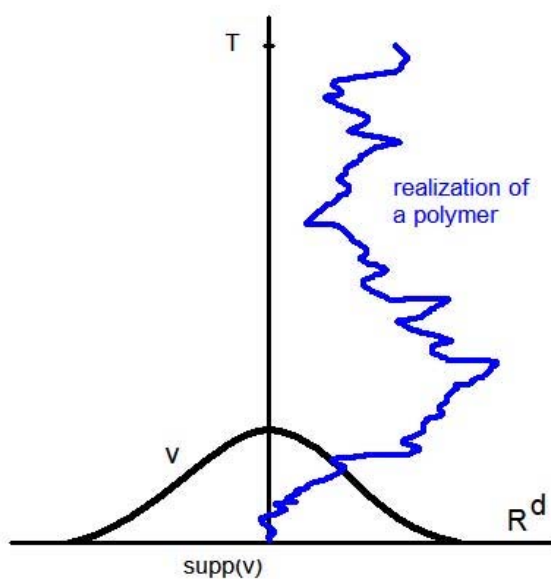
$\beta \geq 0$ - inverse temperature.

$P_{0,T}$ - Wiener measure on $C([0, T], \mathbb{R}^d)$.

Gibbs measure $P_{\beta,T}$ defined by:

$$\frac{dP_{\beta,T}}{dP_{0,T}}(x) = \frac{\exp(\beta \int_0^T v(x(t)) dt)}{Z_{\beta,T}(0)}, \quad x \in C([0, T], \mathbb{R}^d).$$

$Z_{\beta,T}(0)$ - partition function.



First set of questions: What is the typical behavior of $x(t)$, $t \in [0, T]$, when $T \rightarrow \infty$? (for different values of β).

Define p_β as the fundamental solution of the heat equation

$$\begin{aligned}\frac{\partial p_\beta}{\partial t}(t, y, x) &= \frac{1}{2} \Delta_x p_\beta(t, y, x) + \beta v(x) p_\beta(t, y, x), \\ p_\beta(0, y, x) &= \delta(x - y).\end{aligned}$$

For $0 = t_0 < t_1 < t_2 < \dots < t_n \leq T$ and $x_0 = 0$,

$$\begin{aligned}\frac{P_{\beta, T}(x(t_1) \in dx_1, \dots, x(t_n) \in dx_n)}{dx_1 \dots dx_n} &= \\ \frac{\int_{\mathbb{R}^d} \prod_{i=0}^{n-1} p_\beta(t_{i+1} - t_i, x_i, x_{i+1}) p_\beta(T - t_n, x_n, z) dz}{\int_{\mathbb{R}^d} p_\beta(T, 0, z) dz}.\end{aligned}$$

So we are interested in the asymptotics of the solutions (and fundamental solutions) for the parabolic equation with the operator

$$L^\beta u = \frac{1}{2} \Delta_x u + \beta v(x) u.$$

For initial condition $u(0, \cdot) = g$,

$$u(t, \cdot) = -\frac{1}{2\pi i} \int_{\operatorname{Re} \lambda = \lambda_0 + 1} e^{\lambda t} R_\lambda^\beta g d\lambda.$$

Resolvent: $R_\lambda^\beta = (L^\beta - \lambda)^{-1}$.

Resolvent Identity:

$$R_\lambda^\beta = R_\lambda^0 (I + \beta v(x) R_\lambda^0)^{-1}.$$

Analytic and asymptotic properties of R_λ^0 are known (e.g. $R_0(\lambda, x) = \frac{e^{-\sqrt{2\lambda}|x|}}{-2\pi|x|}$, $d = 3$).

Spaces: both sides in the resolvent identity:
 $L^2_{\text{exp}}(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ and $C_{\text{exp}}(\mathbb{R}^d) \rightarrow C(\mathbb{R}^d)$.

$$\|f\|_{L^2_{\text{exp}}(\mathbb{R}^d)} = \left(\int_{\mathbb{R}^d} f^2(x) e^{|x|^2} dx \right)^{\frac{1}{2}}.$$

$$\|f\|_{C_{\text{exp}}(\mathbb{R}^d)} = \sup_{x \in \mathbb{R}^d} (|f(x)| e^{|x|^2}).$$

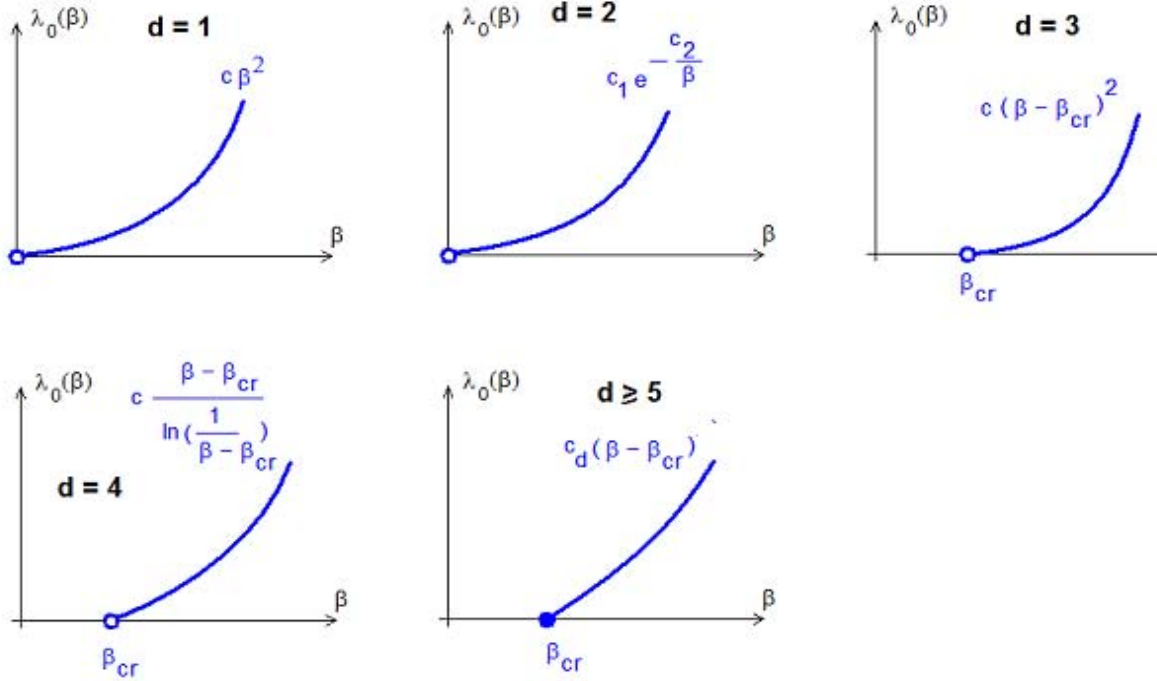
Spectrum:

$$\sigma(H_\beta) = (-\infty, 0] \cup \{\lambda_j(\beta)\}, \quad j \leq N, \quad \lambda_j(\beta) \geq 0.$$

Let $\lambda_0 = \max_j(\lambda_j)$. Then

$$\lim_{T \rightarrow \infty} \frac{\ln Z_{\beta, T}}{T} = \lambda_0(\beta)$$

Lemma: (asymptotics of $\lambda_0(\beta)$ as $\beta \downarrow \beta_{cr}$)



Lemma: – For $\beta > \beta_{cr}$: $\ln Z_{\beta,T} \sim \lambda_0(\beta)T$.
 – For $\beta < \beta_{cr}$: $\lim_{T \rightarrow \infty} Z_{\beta,T} = c(\beta) \sim \frac{c}{\beta - \beta_{cr}}$ (as $\beta \uparrow \beta_{cr}$).

– For $\beta = \beta_{cr}$:

$d = 3$: $Z_{\beta,T} \sim k_3 \sqrt{T}$ as $T \rightarrow \infty$.

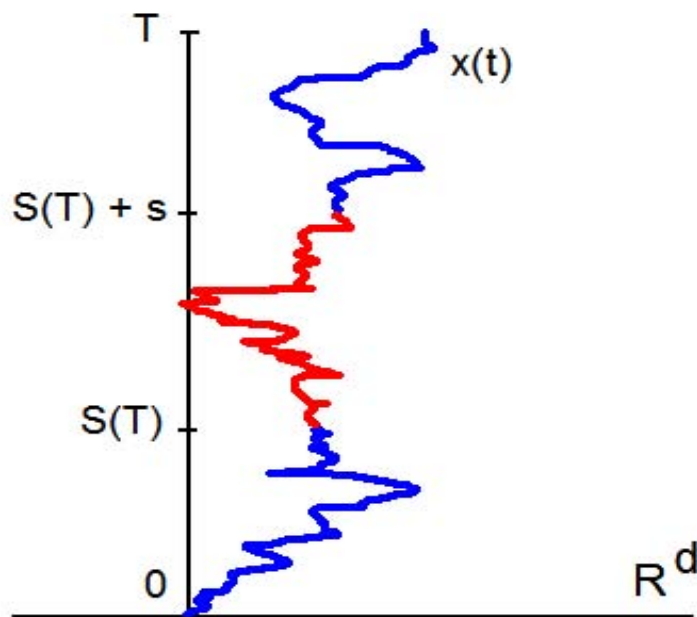
$d = 4$: $Z_{\beta,T} \sim k_4 T / \ln T$ as $T \rightarrow \infty$.

$d \geq 5$: $Z_{\beta,T} \sim k_d T$ as $T \rightarrow \infty$.

Results on the behavior of $x(t)$, $t \in [0, T]$.

Case 1 ($\beta > \beta_{\text{cr}}$). Let $S(T), T - S(T) \rightarrow \infty$, $s > 0$ be fixed.

Let $y^T(t) = x(S(T) + t)$, $0 \leq t \leq s$.



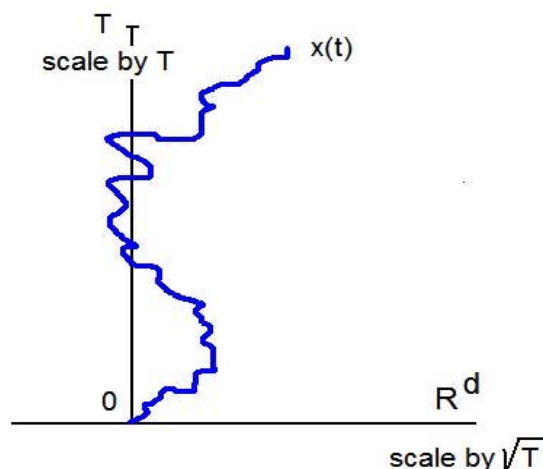
Theorem: $y^T(t)$ converges, as $T \rightarrow \infty$, to a stationary Markov process with finite invariant measure.

Case 2 ($\beta < \beta_{\text{cr}}$). Let $y^T(t) = x(t \cdot T)/\sqrt{T}$, $0 \leq t \leq 1$.

Theorem: $y^T(t)$ converges, as $T \rightarrow \infty$, to d -dimensional Brownian motion.

Case 3 ($\beta = \beta_{\text{cr}}$, $d = 3$).

Let $y^T(t) = x(t \cdot T)/\sqrt{T}$, $0 \leq t \leq 1$.



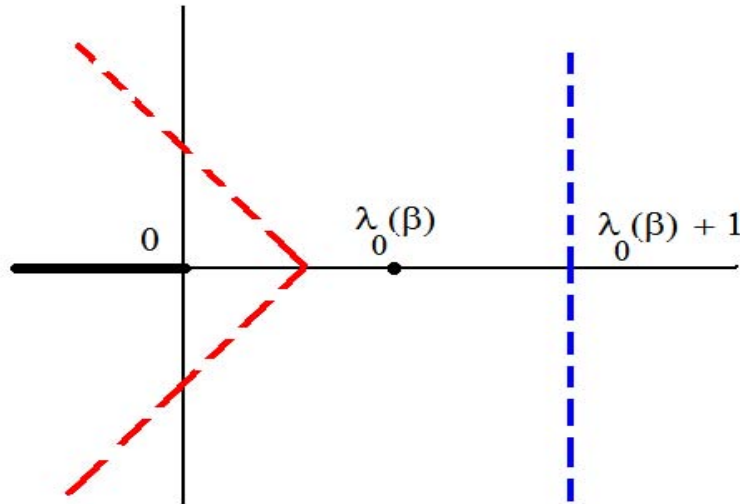
Theorem: $y^T(t)$ converges, as $T \rightarrow \infty$, to a time-dependent rotation-invariant diffusion on \mathbb{R}^d . The process $|y^T(t)|$ converges to a one-dimensional diffusion with reflection at the origin.

Proof outline (Simplest case $\beta > \beta_{\text{cr.}}$)

If u_β solves parabolic eq-n with initial data g ,

$$u_\beta(t, \cdot) = -\frac{1}{2\pi i} \int_{\text{Re}\lambda=\lambda_0+1} e^{\lambda t} R_\lambda^\beta g d\lambda.$$

$$Z_{\beta,t} = \dots, \quad p_\beta(t, y, x) = \dots$$



Let $L_\beta \psi_\beta = \lambda_0(\beta) \psi_\beta$, $\|\psi_\beta\|_{L^2} = 1$, $\psi_\beta \geq 0$.
After moving the contour,

$$u_\beta(t, \cdot) \sim \dots$$

$$Z_{\beta,t}(x) \sim \exp(\lambda_0(\beta)t) \|\psi_\beta\|_{L^1} \psi_\beta(x),$$

$$p_\beta(t, y, x) \sim \exp(\lambda_0(\beta)t) \psi_\beta(y) \psi_\beta(x).$$

Density of $(x(S(T) + t_1), \dots, x(S(T) + t_n))$ is:

$$p_\beta(S(T) + t_1, 0, x_1)p_\beta(t_2 - t_1, x_1, x_2) \times \dots \\ \dots p_\beta(t_n - t_{n-1}, x_{n-1}, x_n)Z_{\beta, T-t_n}(x_n)(Z_{\beta, T}(0))^{-1}. \quad (*)$$

Define:

$$r_\beta(t, y, x) = \frac{p_\beta(t, y, x)\psi_\beta(x)}{\psi_\beta(y)} \exp(-\lambda_0(\beta)t).$$

Then r_β is the transition density of the Markov process with generator

$$\frac{1}{2}\Delta g + \frac{(\nabla \psi_\beta, \nabla g)}{\psi_\beta}.$$

The asymptotics of $(*)$ is:

$$\psi_\beta^2(x_1)r_\beta(t_2 - t_1, x_1, x_2) \cdot \dots \cdot r_\beta(t_n - t_{n-1}, x_{n-1}, x_n).$$

A feature of the case when $\beta = \beta_{\text{cr}}$.

For $|y| \leq \varepsilon^{-1}$, $\varepsilon\sqrt{t} \leq |x| \leq \varepsilon^{-1}\sqrt{t}$:

$$p_\beta(t, y, x) \sim \frac{\varkappa}{|x|\sqrt{t}} \exp(-|x|^2/2t) \psi(y),$$

For $\varepsilon\sqrt{t} \leq |y|, |x| \leq \varepsilon^{-1}\sqrt{t}$:

$$p_\beta(t, y, x) \sim p_0(t, y, x) + \frac{e^{-(|y|+|x|)^2/2t}}{(2\pi)^{3/2}|y||x|\sqrt{t}}.$$

The law of the limiting process does not depend on v ! Its transition density can be written out explicitly.

Part 2: Homopolymers with zero-range potential

Define

$$v_{\gamma}^{\varepsilon} = \left(\frac{\pi^2}{8\varepsilon^2} + \frac{\gamma}{\varepsilon} \right) v\left(\frac{x}{\varepsilon}\right), \quad \|v\|_{L^1(\mathbb{R}^3)} = \frac{4\pi}{3}.$$

Let $P_{\gamma,T}^{x,\varepsilon}$ be the corresponding Gibbs measure ($\beta = 1$ and x is the initial point).

Theorem: For each $\gamma \in \mathbb{R}$ and $T > 0$ there are limits

$$\overline{P}_{\gamma,T}^x = \lim_{\varepsilon \downarrow 0} P_{\gamma,T}^{x,\varepsilon},$$

understood in the sense of weak convergence of measures on $C([0, T], \mathbb{R}^3)$.

How can we describe $\overline{P}_{\gamma,T}^x$?

Theorem ([Albeverio, et. al.]) All the self-adjoint extensions of the Laplacian acting on $C_0^\infty(\mathbb{R}^3 \setminus \{0\})$ to an operator acting on $L^2(\mathbb{R}^3)$ form a one-parameter family \mathcal{L}_γ , $\gamma \in \mathbb{R}$. The spectrum of \mathcal{L}_γ is given by

$$\text{spec}(\mathcal{L}_\gamma) = (-\infty, 0] \cup \left\{ \frac{\gamma^2}{2} \right\}, \quad \gamma > 0,$$

$$\text{spec}(\mathcal{L}_\gamma) = (-\infty, 0], \quad \gamma \leq 0.$$

The kernel of the resolvent of \mathcal{L}_γ is given by

$$R_{\lambda, \gamma}(x, y) = \frac{e^{-\sqrt{2\lambda}|x-y|}}{\pi|x-y|} + \frac{1}{\sqrt{2\lambda} - \gamma} \frac{e^{-\sqrt{2\lambda}(|x|+|y|)}}{2\pi|x||y|},$$

$\lambda \notin \text{spec}(\mathcal{L}_\gamma).$

Define $\bar{p}_\gamma(t, x, y)$ as the kernel of $\exp(t\mathcal{L}_\gamma)$, $t > 0$, and

$$\bar{Z}_\gamma(t, x) = \int_{\mathbb{R}^3} \bar{p}_\gamma(t, x, y) dy,$$

Define the measures $\bar{P}_{\gamma, T}^x$, $x \in \mathbb{R}^3$, via their finite-dimensional distributions

$$\begin{aligned} \bar{P}_{\gamma, T}^x(\omega(t_1) \in A_1, \dots, \omega(t_k) \in A_k) = \\ \bar{Z}_\gamma^{-1}(T, x) \int_{A_1} \dots \int_{A_k} \int_{\mathbb{R}^3} \bar{p}_\gamma(t_1, x, x_1) \dots \\ \dots \bar{p}_\gamma(t_k - t_{k-1}, x_{k-1}, x_k) \bar{p}_\gamma(T - t_k, x_k, y) dy dx_k \dots dx_1, \end{aligned}$$

where $k \geq 1$, $0 \leq t_1 \leq \dots \leq t_k \leq T$ and A_1, \dots, A_k are Borel sets in \mathbb{R}^3 .

Distribution above the critical point

($\gamma = \gamma(T)$ is bounded and $\gamma(T)\sqrt{T} \rightarrow +\infty$ as $T \rightarrow +\infty$):

Let $S(T)$ be such that

$$\lim_{T \rightarrow +\infty} \gamma(T)\sqrt{S(T)} = \lim_{T \rightarrow +\infty} \gamma(T)\sqrt{T - S(T)} = +\infty.$$

Let $s > 0$ be fixed. Consider the process

$$y^T(t) = \gamma(T)\omega(S(T) + t/\gamma^2(T)), \quad 0 \leq t \leq s.$$

Theorem: The distribution of the process $y^T(t)$ with respect to the measure $\bar{\mathbf{P}}_{\gamma(T),T}^x$ converges as $T \rightarrow +\infty$, weakly in the space $C([0, s], \mathbb{R}^3)$, to the distribution of a stationary Markov process.

Distribution near and below the critical point

($\gamma = \gamma(T)$ is such that $\gamma(T)\sqrt{T} \rightarrow \varkappa \in [-\infty, +\infty)$ as $T \rightarrow +\infty$):

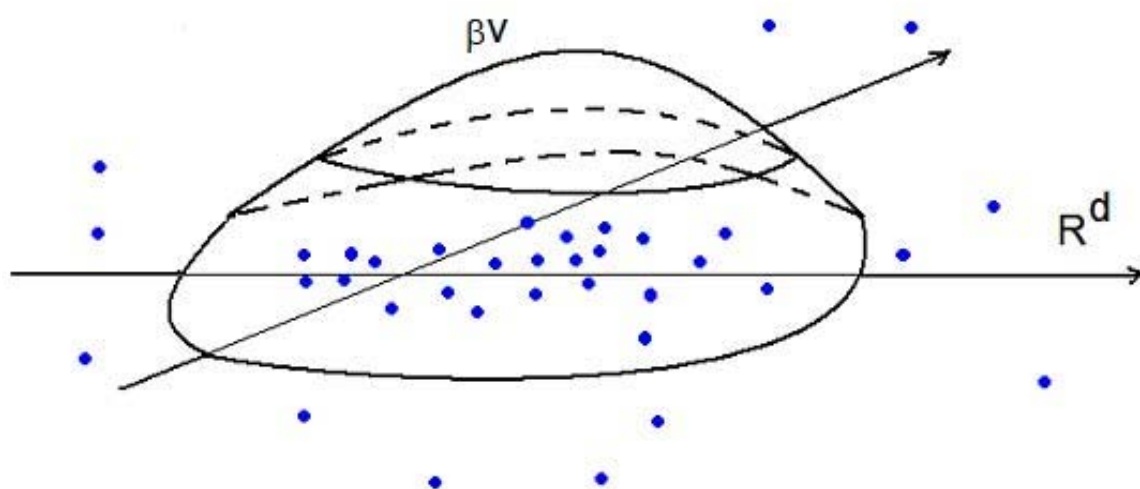
Let $y^T(t) = \omega(tT)/\sqrt{T}$, $0 \leq t \leq 1$.

Theorem: (Self-similarity near the critical point) If $\gamma = \gamma(T)$ is such that $\gamma(T)\sqrt{T} \rightarrow \varkappa \in (-\infty, +\infty)$ as $T \rightarrow +\infty$, then the distribution of the process $y^T(t)$ with respect to the measure $\bar{P}_{\gamma(T),T}^x$ converges as $T \rightarrow +\infty$ to the measure $\bar{P}_{\varkappa,1}^0$.

If $\gamma = \gamma(T)$ is such that $\gamma(T)\sqrt{T} \rightarrow -\infty$ as $T \rightarrow +\infty$, then the distribution of the process $y^T(t)$ with respect to the measure $\bar{P}_{\gamma,T}^x$ converges as $T \rightarrow +\infty$ to the distribution of the 3-dimensional Brownian motion.

Part 3: Branching Diffusions

v - intensity of branching.



Initially - one particle located at $x \in \mathbb{R}^d$. Goal - to describe the distribution of particles when t is large.

Again, look at the operator

$$L^\beta u(x) = \frac{1}{2} \Delta u(x) + \beta v(x) u(x).$$

Theorem: For $\beta > \beta_{\text{cr}}$ the number of particles in a given domain U at time t has the asymptotics (as $t \rightarrow \infty$):

$$n_t(U) \sim e^{\lambda_0(\beta)t} \xi_\beta^x \int_U \psi_\beta(y) dy,$$

For $\beta < \beta_{\text{cr}}$:

$$n_t(\mathbb{R}^d) \sim \eta_\beta^x.$$

Equations on correlation functions

$\rho_1(t, x, y_1)$ - particle density

$\rho_n(t, x, y_1, \dots, y_n)$ - higher order correlation functions.

For fixed y_1, \dots, y_n , they satisfy the equations

$$\partial_t \rho_1(t, x, y_1) = \frac{1}{2} \Delta \rho_1(t, x, y_1) + \beta v(x) \rho_1(t, x, y_1),$$

$$\rho_1(0, x, y_1) = \delta_{y_1}(x).$$

$$\begin{aligned} \partial_t \rho_n(t, x, y_1, \dots, y_n) = & \frac{1}{2} \Delta \rho_n(t, x, y_1, \dots, y_n) + \\ & + \beta v(x) (\rho_n(t, x, y_1, \dots, y_n) + H_n(t, x, y_1, \dots, y_n)), \end{aligned}$$

$$\rho_n(0, x, y_1, \dots, y_n) \equiv 0.$$

Here

$$H_n = \sum_{U \subset Y, U \neq \emptyset} \rho_{|U|}(t, x, U) \rho_{n-|U|}(t, x, Y \setminus U).$$

Let r be the distance from $\lambda_0(\beta)$ to the rest of the spectrum.

Let $P_t : C_{\text{exp}} \rightarrow C$ be the operator that maps the initial function g to the solution of $u'_t = L^\beta u$.

Lemma 1: Let $K \subset \mathbb{R}^d$ be a compact set. For each $\varepsilon \in (0, r)$, the function $\rho_1(t, x, y)$ satisfies

$$\rho_1(t, x, y) = \exp(\lambda_0 t) \psi_\beta(x) \psi_\beta(y) + q(t, x, y),$$

where

$$\sup_{x \in K} |q(t, x, y)| \leq A_\varepsilon \exp((\lambda_0 - \varepsilon)t - |y| \sqrt{2(\lambda_0 - \varepsilon)}).$$

for $t \geq 1/2$.

Lemma 2 Let $K \subset \mathbb{R}^d$ be a compact set. For each $\varepsilon \in (0, r)$, the function ρ_n satisfies

$$\rho_n(t, x, y_1, \dots, y_n) = \exp(n\lambda_0 t) f_n(x) \psi_\beta(y_1) \cdots \psi_\beta(y_n) \\ + q_n(t, x, y_1, \dots, y_n),$$

where

$$\sup_{x \in K} |q_n(t, x, y_1, \dots, y_n)| \leq A_\varepsilon^n \exp(n\lambda_0 t) \Pi_\varepsilon^n(t, y_1, \dots, y_n).$$

for $t \geq 1/2$.

The functions f_1, f_2, \dots are defined inductively:
 $f_1 = \psi_\beta$ and

$$f_n = \beta \sum_{k=1}^{n-1} \frac{n!}{k!(n-k)!} I_n(v f_k f_{n-k}), \quad n \geq 2,$$

$$\text{where} \quad I_n(g) := \int_0^\infty \exp(-n\lambda_0 s) P_s g ds.$$

Π_ε^n - decays sufficiently fast in t, y_1, \dots, y_n .

Proof of the Theorem (case $\beta > \beta_{\text{cr}}$)

Look at the asymptotics of the moments.

$$\mathbb{E}(n_t^x(U))^n = \int_U \dots \int_U \rho_n(t, x, y_1, \dots, y_n) dy_1 \dots dy_n.$$

Divide by $\exp(n\lambda_0 t)$ and check that the limiting quantities satisfy the Carleman condition.

Sufficient to check that

$$\sum_{n=1}^{\infty} \left(\frac{1}{f_n(x)} \right)^{\frac{1}{2n}} = \infty. \quad (*)$$

From the properties of I_n it follows that $\exists A$ s.t.:

$$\|f_n\|_C \leq A \sum_{k=1}^{n-1} \frac{(n-1)!}{k!(n-k)!} \|f_k\|_C \|f_{n-k}\|_C, \quad n \geq 2,$$

$$\|f_1\|_C \leq A.$$

From here, by induction on n it follows that $\|f_n\|_C \leq A^{2n-1} n!$, which in turn implies $(*)$ since $n! \leq ((n+1)/2)^n$.