Correlation decay for particle systems on the real line interacting via a Lennard-Jones type potential

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Motivation

We study one dimensional systems interacting via a Lennard-Jones type potential with hard core, and introduce the two different setting in which correlation decay can occur: the Lagrangian picture and the Eulerian picture (see Figure 1). Notably, in the Lagrangian picture the system can be seen as a lattice system with continuous (positive) spin. We try to establish a connection between the two picture by developing techniques to translate the quantitative results for Lagrangian picture to that for Eulerian picture.

Infinite Volume Gibbs Measure

Consider N particles with positions $x_1, \dots, x_N$ and inter-particle spacing $z_j = x_{j+1} - x_j$. The energy of the system interacting via the aforementioned potential, truncated to next-nearest-neighbour:

$$E_N(z_1, \dots, z_{N-1}) = \sum_{i=1}^{N-1} v(z_i) + \sum_{i=1}^{N-2} v(z_i + z_{i+1}), \tag{1}$$

where $v : [0, \infty) \to \mathbb{R},\ v(x) = 1/(x - r_{hc})^{12} - 1/(x - r_{hc})^6$ if $x > r_{hc}$ and $v(x) = \infty$ otherwise.

Gibbs measure (on $\mathbb{R}_+^{N-1}$)in constant pressure ensemble:

$$\mu_{N,\beta}(A) = \frac{1}{Z_{N,\beta}} \int_A \exp\left(-\beta(E_N((z_1, \dots, z_{N-1})) + p\sum_{i=1}^{N-1} z_i)\right) dz_1 \dots dz_{N-1}. \tag{2}$$

There exists a unique infinite volume Gibbs measure μ_β on $\mathbb{R}_+^{\mathbb{Z}}$, such that for all $k \in \mathbb{N}$, every bounded continuous test function $f \in C_b(\mathbb{R}_+^k)$, and all sequences i_N with $i_N \to \infty$ and $N - i_N \to \infty$,

$$\lim_{N\to\infty} \int_{\mathbb{R}_+^{N-1}} f(z_{i_N+1}, \dots, z_{i_N+k}) d\mu_{N,\beta}(z_1, \dots, z_{N-1}) = \int_{\mathbb{R}_+^{\mathbb{Z}}} f(z_1, \dots, z_k) d\mu_\beta((z_j)_{j\in\mathbb{Z}}). \tag{3}$$

This Gibbs measure μ_β is shift invariant.

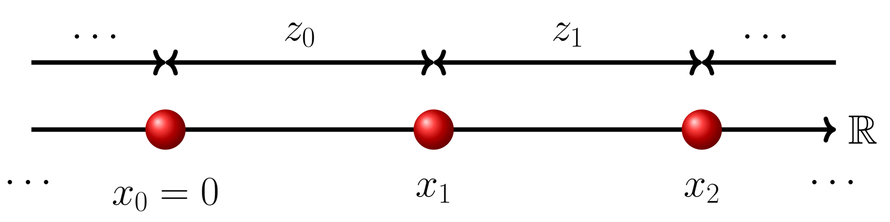

Figure 1. The configuration parametrized in two different ways: it is described either by position of one particle together with a doubly infinite sequence of spacings $\{z_i\}_{i\in\mathbb{Z}} \in \mathbb{R}_+^{\mathbb{Z}}$; or it is described straightforwardly with a doubly infinite increasing sequence of positions, $\{x_i\}_{i\in\mathbb{Z}} \in \mathbb{R}^{\mathbb{Z}}$.

Gaussian Approximation

Approximating energy eq.(1) to second order gives Gaussian transition kernel, and the Markov chain $\{Z'_n\}_{n\in\mathbb{N}} = \{Z_n - a\}_{n\in\mathbb{N}}$ is a first order autoregressive process,

$$Z'_n = \alpha Z'_{n-1} + \eta_n, \tag{4}$$

where a is the distance between particles in ground state, $\alpha \in (0, 1)$ is a constant and η_n are i.i.d. normal distributed noise with a fixed variance.

Lemma

For the Gaussian approximation, $\int_0^\infty e^{\theta x} G(dx) < \infty$ for some $\theta > 0$.

Sketch of Proof:

First note that

$$1 - G(u) = \mathbb{P}(\sum_{i=0}^{\tau-1} Z'_i + \tau a \geq u) \leq \mathbb{P}(\sum_{i=0}^{\tau-1} Z'_i \geq \frac{u}{2}, \tau a \leq \frac{u}{2}) + \mathbb{P}(\tau a \geq \frac{u}{2}). \tag{5}$$

Define $d(x) = -\frac{1}{\log\alpha} \log\frac{|x|}{\alpha r}$ with some $r > 0$, we have

$$\mathbb{P}(\tau \geq v) \leq \mathbb{P}(d(Z_0) \geq v/3) + \mathbb{P}(\sum_{i=1}^{u} d(|\eta_i| + r) \geq v/3) + \mathbb{P}(\gamma \geq v/3), \tag{6}$$

where γ is a geometric random variable with parameter depending on r and variance of η. The lemma now follows by using Chernoff bounds on the first term in RHS of eq.(5) and second term in RHS of eq.(6).

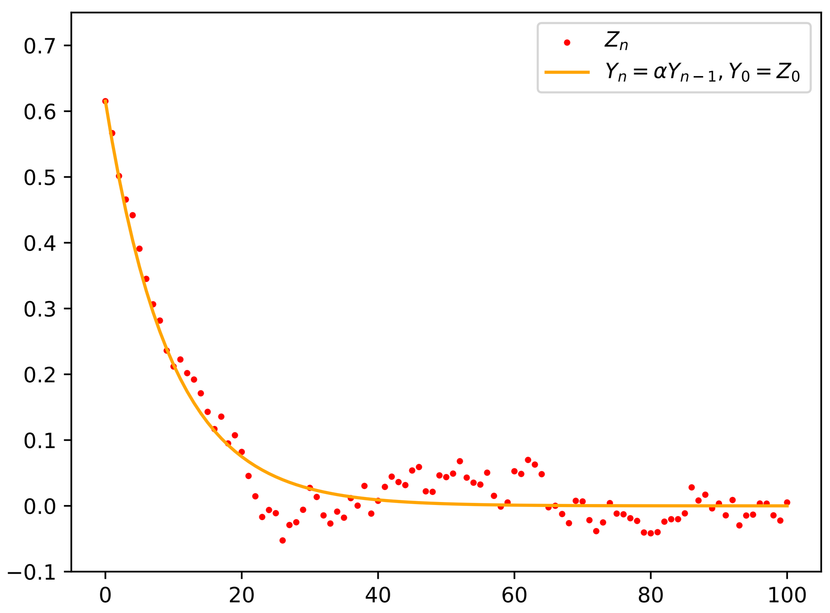

Figure 2. A realization of the first order auto-regression process with some initial value Z_0.

Question and Answer

Suppose that for some $c > 0$,

$$\mathbb{E}[Z_0 Z_n] - \mathbb{E}[Z_0]\mathbb{E}[Z_n] = \mathcal{O}(e^{-cn}). \tag{7}$$

Under what conditions do we have that there exists some $c' > 0$, such that for any Borel sets A, B,

$$\mathbb{E}[N_A N_B] - \mathbb{E}[N_A]\mathbb{E}[N_B] = \mathcal{O}(e^{-c' d(A,B)}), \tag{8}$$

where N_A, N_B are number of particles in A, B respectively?

Shift operator T_t: for any measurable set B, $T_t B := \{y + t \mid y \in B\}$.

Theorem

Suppose $\int_0^\infty e^{\theta x} G(dx) < \infty$, $\int_0^\infty e^{\omega x} G'(dx) < \infty$ for some $\theta, \omega > 0$ (distribution of the embedded renewal process has finite exponential moment). Suppose $A, B \subset \mathbb{R}$ are bounded intervals, $t^* := \inf\{t \mid A \cap T_u B = \emptyset\ \forall u > t\}$. Then there exists $\xi > 0$ such that for all $t > t^*$, $\mathrm{Cov}(N_A, N_{T_t B}) = \mathcal{O}(e^{-\xi t})$.

Exponential Decay via Renewal Theory

The chain of atoms (doubly infinite sequence of spacings) under the measure μ_β is a doubly infinite Markov Chain $\{Z_n\}_{n\in\mathbb{Z}}$ on $\mathbb{R}_+$, with the transition kernel

$$P_\beta(x, dy) := \frac{1}{\Lambda_0(\beta)\phi_\beta(x)} K_\beta(x, y)\phi(y) dy, \tag{9}$$

where K_β is a suitably defined transfer operator, $\Lambda_0(\beta)$ and ϕ_β are its largest eigenvalue and the corresponding eigenfunction respectively. This Markov chain has its invariant probability measure as the initial measure $\rho_\beta(x)dx$, where $\rho_\beta(x) = \frac{1}{c}(\phi_\beta(x))^2$[5].

This Markov chain is *Harris recurrent*: there exists a non-trivial σ-finite measure φ such that

$$\varphi(B) > 0 \Rightarrow \forall x \quad \mathbb{P}_x(\{Z_n\}_n \text{ visits } B \text{ infinitely often}) = 1. \tag{10}$$

There is an *embedded renewal process* with some distribution G.

Suppose $D = [0, \zeta]$, $0 < \zeta < \infty$, $t \leq 0$, the function

$$Z(t) = \mathbb{E}_\nu[\#\{n : X_n \in T_{t-\zeta} D\}], \tag{11}$$

where $X_n = \sum_{i=0}^{n-1} Z_i$, satisfies the *renewal equation*

$$Z(t) = z(t) + \int_0^t Z(t - u) G(du) \tag{12}$$

for some suitable function z. Renewal theory[1] implies

Lemma

Suppose $\int_0^\infty e^{\theta x} G(dx) < \infty$ for some $\theta > 0$. Then there exists $\epsilon > 0$ such that

$$Z(t) = \frac{|D|}{\mathbb{E}_\rho[Z_0]} + \mathcal{O}(e^{-\epsilon t}). \tag{13}$$

Switching Pictures via Palm Theory

Let $(\mathcal{N}, \mathcal{B}(\mathcal{N}))$ be the space of locally finite counting measure on $\mathbb{R}$, and $\mathcal{N}_0 := \{N \in \mathcal{N} \mid N(0) = 1\}$.

Simple one-to-one correspondence, Ξ between the space $(\mathcal{N}_0, \mathcal{B}(\mathcal{N}_0))$ and $(\mathbb{R}_+^{\mathbb{Z}}, \mathcal{B}(\mathbb{R}_+^{\mathbb{Z}}))$: let $\{\dots, x_{-1}, x_0 = 0, x_1, \dots\}$ with $x_i < x_{i+1}$ for all $i \in \mathbb{Z}$,

$$\mathcal{N}_0 \ni N = \sum_{i\in\mathbb{Z}} \delta_{x_i} \mapsto \Xi N = \{z_{i-1} = x_i - x_{i-1} \mid i \in \mathbb{Z}\} \in \mathbb{R}_+^{\mathbb{Z}}. \tag{14}$$

The point process $\Phi^0 = \Xi^{-1} = \delta_0 + \sum_{i\in\mathbb{Z}\setminus\{0\}} \delta_{X_i}$ has distribution $\mathbb{P}^0 = \mu_\beta \circ (\Phi^0)^{-1}$.

Ryll-Nardzewski and Slivnyak inversion formula [3]: There exists a unique non-null translation invariant point process Φ which has Φ^0 as its Palm distribution.

Number operator for a Borel set A: $N_A(\cdot) = \Phi(\cdot)(A)$.

For stationary point process, *second factorial moment measure* $M_{\Phi^{(2)}}$ can be determined using the *reduced second moment measure* $\mathcal{K}(E) = \mathbb{E}^0[\Phi^!(E)]$, $\Phi^! = \Phi - \delta_0$, as [2]

$$M_{\Phi^{(2)}}(A \times T_t B) = \lambda \int_A \mathcal{K}(T_{t-x} B) dx. \tag{15}$$

The result follows from the observations that $\mathbb{E}_\rho[Z_0] = \lambda^{-1}$ and for $t > |B|$,

$$\mathcal{K}(T_{t-|B|} D) = Z_\rho(t). \tag{16}$$

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