

On the identifiability of interaction functions in systems of interacting particles

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Abstract

We address a fundamental issue in the nonparametric inference for systems of interacting particles: the identifiability of the interaction functions. We prove that the interaction functions are identifiable for a class of first-order stochastic systems, including linear systems and nonlinear systems with stationary distributions in the decentralized directions. The identifiability, in terms of a coercivity condition, is equivalent to the strict positiveness of integral operators arisen from the nonparametric regression. We then prove the positiveness based on series representations of the associated integral kernels and Müntz type theorems for the completeness of polynomials on an unbounded domain.

Keywords: interacting particle systems, nonparametric regression, positive definite kernel, positive operator, identifiability

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1. Introduction

Dynamical systems of interacting particles or agents are widely used in many areas in science and engineering, such as physics [1], biology [2], social science [3, 4], and we refer to [5, 6] for reviews. With the recent advancement of technology in data collection and computation, inference of such systems from data has been attracting an increasing attention [7, 8, 9]. In general, such systems are high-dimensional and there is no simple parametric form, so the inference tends to be computationally infeasible due to the curse of dimensionality. An exception is when there is a symmetric structure, such that one only needs to estimate a low-dimensional interaction function, for example, depending on only the pairwise distances between particles [10, 11]. However, a fundamental challenge arises: the interaction function may be non-identifiable, because its values are under-determined even with perfect trajectory data. To ensure the identifiability of the interaction function, a coercivity condition is introduced in [10, 11]. In this study, we prove that the coercivity condition holds true for linear systems, and a class of three-particle nonlinear systems with stationary distributions.

More precisely, consider a first-order stochastic gradient system of interacting particles:

$$d\mathbf{X}_i^t = \frac{1}{N} \sum_{1 \leq j \leq N, j \neq i} \phi(|\mathbf{X}_j^t - \mathbf{X}_i^t|) \frac{\mathbf{X}_j^t - \mathbf{X}_i^t}{|\mathbf{X}_j^t - \mathbf{X}_i^t|} dt + \sigma d\mathbf{B}_i^t, \quad \text{for } i = 1, \dots, N, \quad (1.1)$$

where $\mathbf{X}_i^t \in \mathbb{R}^d$ represents the position of particle i at time t , $\{\mathbf{B}_i^t\}_{i=1}^N$ are independent Brownian motions representing the random environment, and σ is a positive constant representing the strength of the noise. Without loss of generality, we assume $\sigma = 1$ in (1.1). Hereafter $|\cdot|$ denote the Euclidean norm of vectors. We assume that the agents are of the same type, with a function $\phi : \mathbb{R}^+ = [0, \infty) \rightarrow \mathbb{R}$ modeling the pairwise interaction between particles, which is referred to as the *interaction function*.

In the inference of the interaction function by nonparametric regression, the following coercivity condition is found to ensure identifiability [10, 11]: for any compact subspace $\mathcal{H} \subset L^2(\rho_t)$, where ρ_t denotes the probability density function of $|\mathbf{r}_{ji}^t|$ with $\mathbf{r}_{ji}^t := \mathbf{X}_j^t - \mathbf{X}_i^t$,

$$c_{\mathcal{H},N}(t) := \inf_{h \in \mathcal{H} \cap \partial B_1} \mathbb{E} \left[h(|\mathbf{r}_{12}^t|) h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t| |\mathbf{r}_{13}^t|} \right] > 0, \quad (1.2)$$

where ∂B_1 denotes the unit sphere in $L^2(\rho_t)$.

We prove coercivity condition for systems with a class of interaction functions, particularly for $\phi(r) = r$ which leads to linear systems, and for three-particle nonlinear systems with $\phi(r)$ dominated by r^α for $\alpha \in (0, 1]$ and with a stationary distribution. We show first that the coercivity condition is equivalent to the positiveness of an integral operator arisen from the expectation in Eq. (1.2). More precisely, note that

$$\mathbb{E} \left[h(|\mathbf{r}_{12}^t|) h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t| |\mathbf{r}_{13}^t|} \right] = \int_0^\infty \int_0^\infty h(r) h(s) K_t(r, s) dr ds$$

where the integral kernel $K_t : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}$ with $t \in [0, T]$ is defined as

$$K_t(r, s) := (rs)^{d-1} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p_t(r\xi, s\eta) d\xi d\eta, \quad (1.3)$$

with $p_t(u, v)$ denoting the density function of the random vector $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$ and S^{d-1} denoting the unit sphere in \mathbb{R}^d . Thus the coercivity condition is equivalent to that the integral operator associated with the integral kernel K_t is strictly positive. Then, to prove the strict positiveness of the operator, we introduce a series representation of the integral kernel and resort to a Müntz type theorem on the completeness in $L^2(\rho_t)$ of polynomials with even degrees (Section 3). In particular, in the treatment of nonlinear systems, we develop a “comparison to a Gaussian kernel” technique (Section 4.2, 4.3) to prove the strictly positiveness for a large class of interaction kernels.

In this study, we consider only regular interaction kernels that lead to continuous drift terms, and thus a global strong solution to the system. Many directions are beyond the scope of this study and will be left for future works: first-order nonlinear systems with more general interactions kernels that are regular [9, 10]

or singular [12, 13] or starting from non-stationary distributions, second-order systems and systems with multiple types of particles or agents [11].

Positive definite integral kernels play an increasingly prominent role in many applications in science, in particular in statistical learning theory and in reproducing kernel Hilbert space representations [14, 15, 16]. Our results provides a new class of positive definite integral kernels, and our technique of comparison to a Gaussian kernel may be used to establish identifiability in other learning problems.

The organization of the paper is as follows: in Section 2, we introduce the coercivity conditions in inference, and establish the connections between the coercivity conditions and positive integral operators. In Section 3 we prove the coercivity condition for linear systems and Section 4 is devoted to a class of three-particle nonlinear systems with stationary distributions. We list in Section 5 the preliminaries for the proofs, such as the properties of positive definite kernels, a Müntz-type theorem on half-line, and a stationary measure for gradient systems.

2. The coercivity conditions and strictly positive integral operators

In vector format, we can write the system (1.1) as

$$d\mathbf{X}^t = -\nabla J_\phi(\mathbf{X}^t)dt + d\mathbf{B}^t \quad (2.1)$$

where $\mathbf{X}^t := (\mathbf{X}_i^t)_{i=1}^N \in \mathbb{R}^{Nd}$, and the potential function $J_\phi : \mathbb{R}^{Nd} \rightarrow \mathbb{R}$ reads

$$J_\phi(\mathbf{X}) = \frac{1}{2N} \sum_{i,j=1, j \neq i}^N \Phi(|\mathbf{x}_i - \mathbf{x}_j|), \quad \mathbf{x} \in \mathbb{R}^{Nd}, \text{ with } \Phi'(r) = \phi(r). \quad (2.2)$$

In this study, we assume that $\Phi \in C^1(\mathbb{R}^+, \mathbb{R}^+)$ such that $p(\mathbf{X}) := e^{J_\phi(\mathbf{X})}$ satisfying

(H1) $\sqrt{p} \in W_{loc}^{1,2}(\mathbb{R}^{Nd}, d\mathbf{X})$ with $d\mathbf{X}$ being the Lebesgue measure;

(H2) $|\nabla J_\phi(\mathbf{X})| \in L^{Nd+\epsilon}(\mathbb{R}^{Nd}, p)$ for some $\epsilon > 0$.

Then, there exists a diffusion process satisfying the above equation (see [17]). In particular, the diffusion operator leads to a strongly continuous semigroup on $L^2(\mathbb{R}^{Nd}, p)$. Further, we assume that the initial condition satisfies a distribution that is exchangeable and absolutely continuous with respect to the Lebesgue measure.

2.1. The coercivity condition in nonparametric inference

Given observations of sample trajectories $\{\mathbf{X}^{[0,T],m}\}_{m=1}^M$ for the system with interaction function φ_{true} , one obtains an estimator of the interaction function by minimizing the likelihood ratio of these trajectories over a hypothesis space \mathcal{H} :

$$\hat{\varphi}_M := \arg \min_{\varphi \in \mathcal{H}} \mathcal{E}^M(\varphi), \quad \text{with } \mathcal{E}^M(\varphi) := \frac{1}{M} \sum_{m=1}^M \mathcal{E}_{\mathbf{X}^{[0,T],m}}(\varphi)$$

where $\mathcal{E}_{\mathbf{X}^{[0,T],m}}(\varphi)$ denotes the likelihood ratio of the trajectory $\mathbf{X}^{[0,T],m}$ and is given by the Girsanov theorem (see e.g. [18])

$$\mathcal{E}_{\mathbf{X}^{[0,T]}}(\varphi) = \frac{1}{2TN} \int_0^T (\|\nabla J_\varphi(\mathbf{X}^t)\|^2 dt + 2\langle \nabla J_\varphi(\mathbf{X}^t), d\mathbf{X}^t \rangle).$$

The function space of learning is $L^2(\bar{\rho}_T)$. Here $\bar{\rho}_T$ is the distribution of all the pairwise distances $\{|\mathbf{X}_i^t - \mathbf{X}_j^t|, t \in [0, T]\}_{i,j}$, and by the exchangeability of the distribution of \mathbf{X}^t (which implies that all the pairs $\mathbf{X}_i^t - \mathbf{X}_j^t$ have the same distribution), it can be written as

$$\bar{\rho}_T(r) = \frac{1}{T} \int_0^T \rho_t(r) dt, \quad \text{with } \rho_t(r) = \mathbb{E}[\delta(|\mathbf{X}_i^t - \mathbf{X}_j^t| - r)]. \quad (2.3)$$

Here $\rho_t(r)$ denotes the probability density function of $|\mathbf{X}_i^t - \mathbf{X}_j^t|$. It is straightforward to show that it exists and is independent of (i, j) by exchangeability, as long as the initial distribution μ_0 is exchangeable and absolutely continuous with respect to the Lebesgue measure.

In proving the consistency of the estimator (convergence to the truth as data size $M \rightarrow \infty$), one controls the error of an estimator φ by the discrepancy between the empirical likelihood ratios, $\mathcal{E}^M(\varphi) - \mathcal{E}^M(\varphi_{true})$, which converges to $\mathbb{E}\mathcal{E}_{\mathbf{X}^{[0,T]}}(\varphi) - \mathbb{E}\mathcal{E}_{\mathbf{X}^{[0,T]}}(\varphi_{true})$ by the Law of Large Numbers. Noting that $d\mathbf{X}_t = -\nabla J_{\varphi_{true}}(\mathbf{X}_t)dt + d\mathbf{B}_t$ and that J_φ is linear in φ , we have

$$\begin{aligned} & \|\nabla J_\varphi(\mathbf{X}^t)\|^2 dt + 2\langle \nabla J_\varphi(\mathbf{X}^t), d\mathbf{X}^t \rangle \\ &= \|\nabla J_\varphi(\mathbf{X}^t)\|^2 dt - 2\langle \nabla J_\varphi(\mathbf{X}^t), \nabla J_{\varphi_{true}}(\mathbf{X}_t) \rangle dt + \langle \nabla J_\varphi(\mathbf{X}^t), d\mathbf{B}^t \rangle \\ &= \|\nabla J_{\varphi - \varphi_{true}}(\mathbf{X}^t)\|^2 dt - \|\nabla J_{\varphi_{true}}(\mathbf{X}^t)\|^2 dt + \langle \nabla J_\varphi(\mathbf{X}^t), d\mathbf{B}^t \rangle, \end{aligned}$$

and hence

$$\mathbb{E}\mathcal{E}_{\mathbf{X}^{[0,T]}}(\varphi) = \frac{1}{2TN} \int_0^T \mathbb{E}\|\nabla J_{\varphi - \varphi_{true}}(\mathbf{X}^t)\|^2 dt + \mathbb{E}\mathcal{E}_{\mathbf{X}^{[0,T]}}(\varphi_{true}).$$

A control on the error of the estimator $h = \varphi - \varphi_{true}$, can then be realized, if the following inequality holds true

$$\frac{1}{TN} \int_0^T \mathbb{E}\|\nabla J_h(\mathbf{X}^t)\|^2 dt \geq C_{\mathcal{H}} \|h\|_{L^2(\bar{\rho}_T)}^2 \quad (2.4)$$

for some constant $C_{\mathcal{H}} > 0$ for all $h \in \mathcal{H}$.

Also, by exchangeability, with notation $\mathbf{r}_{ji}^t = \mathbf{X}_j^t - \mathbf{X}_i^t$, we have

$$\frac{1}{N} \mathbb{E}\|\nabla J_h(\mathbf{X}^t)\|^2 = \sum_{i=1}^N \frac{1}{N^3} \sum_{\substack{j,k=1, \\ j \neq i, k \neq i}}^N \underbrace{\mathbb{E}[h(|\mathbf{r}_{ji}^t|)h(|\mathbf{r}_{ki}^t|) \frac{\langle \mathbf{r}_{ji}^t, \mathbf{r}_{ki}^t \rangle}{|\mathbf{r}_{ji}^t||\mathbf{r}_{ki}^t|}]}_{I_{ijk}} = \frac{(N-1)[(N-2)I_{123} + I_{122}]}{N^2},$$

where the equality follows from that $I(ijk) = I(123)$ for all triplets $\{(i, j, k), j \neq i, k \neq i, j \neq k\}$, contributing $N(N-1)(N-2)$ copies of $I(123)$; and that $I(ijk) = I(122)$ for all for all triplets $\{(i, j, k), j = k \neq i\}$, contributing $N(N-1)$ copies of I_{122} . Note that $I_{122} = \mathbb{E}[h(|U|)^2]$. Therefore, Eq. (2.4) is equivalent to

$$\frac{1}{T} \int_0^T \mathbb{E}[h(|\mathbf{r}_{12}^t|)h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}](t) dt \geq C_{N,T} \frac{1}{T} \int_0^T \mathbb{E}[|h(r_{12})|^2] dt$$

with $C_{N,T} = \frac{N^2}{(N-1)(N-2)}(C_{\mathcal{H}} - \frac{N-1}{N^2})$.

Since in practice the true interaction function and estimators are in a compact subspace $\mathcal{H} \subset L^2(\bar{\rho}_T)$, e.g. $\mathcal{H} = W_{loc}^{1,\infty}(\mathbb{R}^+)$, the above inequality motivates the following **coercivity condition**, so as to ensure the convergence of the estimator.

Definition 2.1 (Coercivity condition on a time interval). *The dynamical system (1.1) on $[0, T]$ with initial condition \mathbf{X}^0 is said to satisfy the coercivity condition on a compact subspace $\mathcal{H} \subset L^2(\bar{\rho}_T)$, with $\bar{\rho}_T$ defined in (2.3), if*

$$c_{\mathcal{H},T} := \inf_{h \in \mathcal{H}, \|h\|_{L^2(\bar{\rho}_T)}=1} \frac{1}{T} \int_0^T \mathbb{E}[h(|\mathbf{r}_{12}^t|)h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}] dt > 0, \quad (2.5)$$

where $\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t$. If the coercivity condition holds true on every compact subspace $\mathcal{H} \subset L^2(\bar{\rho}_T)$, we say the system satisfies the coercivity condition.

We remark that the above coercivity constant $c_{\mathcal{H},T}$ is independent of N , the number of particles in the system. This suggests the interaction function can be identified from the mean field equation of the system when the number of particles are large [19].

The above coercivity condition involves the average-in-time density $\bar{\rho}_T$, which is difficult to track in general. It is more convenient to consider a single-time version.

Definition 2.2 (Coercivity condition at time t). The dynamical system (1.1) with initial condition \mathbf{X}^0 is said to satisfy the coercivity condition at time t on a compact subspace $\mathcal{H} \subset L^2(\rho_t)$, where ρ_t is defined in (2.3), if

$$c_{\mathcal{H}}(t) := \inf_{h \in \mathcal{H}, \|h\|_{L^2(\rho_t)}=1} \mathbb{E}[h(|\mathbf{r}_{12}^t|)h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}] > 0, \quad (2.6)$$

where $\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t$. If the coercivity condition holds true on every compact subspace $\mathcal{H} \subset L^2(\rho_t)$, we say the system satisfies the coercivity condition at time t .

85 The coercivity condition at a single time indicates that the interaction function can be learned from a large size of samples at a single time. This explains the observation in [10, 11] that the kernel can be learned from multiple short-time trajectories.

2.2. Relation to strictly positive integral operators

We show in this subsection that the coercivity condition is equivalent to the strict positivity of related 90 integral operators on $L^2(\bar{\rho}_T)$ or $L^2(\rho_t)$.

Recall that a linear operator Q on a Hilbert space H is *positive* if $\langle Qf, f \rangle \geq 0$ for any $f \in H$. It is said to be *strictly positive* if it is positive and $\langle Qf, f \rangle = 0$ implies that $f = 0$.

Proposition 2.3. The system (1.1) on $[0, T]$ with initial condition \mathbf{X}^0 satisfies the coercivity condition if and only if the integral operator associated with the kernel

$$\bar{K}_T(r, s) := \frac{1}{\bar{\rho}_T(r)\bar{\rho}_T(s)} (rs)^{d-1} \frac{1}{T} \int_0^T \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p_t(r\xi, s\eta) d\xi d\eta dt \quad (2.7)$$

is strictly positive on $L^2(\bar{\rho}_T)$, where $p_t(u, v)$ denotes the probability density function of the random vector $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$.

Proof. Let \bar{Q}_T denote the integral operator associated with $\bar{K}_T(r, s)$ on $L^2(\bar{\rho}_T)$, that is,

$$[\bar{Q}_T h](r) = \int \bar{K}_T(r, s) h(s) \bar{\rho}_T(s) ds. \quad (2.8)$$

Note that for any $h, g \in L^2(\bar{\rho}_T)$,

$$\begin{aligned} \langle \bar{Q}_T h, g \rangle &= \frac{1}{T} \int_0^T \mathbb{E}[h(|\mathbf{r}_{12}^t|)g(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}] dt \\ &\leq \frac{1}{T} \int_0^T \mathbb{E}[h(|\mathbf{r}_{12}^t|)g(|\mathbf{r}_{13}^t|)] dt \leq \|h\|_{L^2(\bar{\rho}_T)} \|g\|_{L^2(\bar{\rho}_T)}. \end{aligned}$$

95 Thus, \bar{Q}_T is a symmetric bounded linear operator on $L^2(\bar{\rho}_T)$.

By definition, the coercivity condition is equivalent to that

$$\inf_{h \in \mathcal{H}, \|h\|_{L^2(\bar{\rho}_T)}=1} \langle \bar{Q}_T h, h \rangle > 0$$

for each compact subspace $\mathcal{H} \subset L^2(\bar{\rho}_T)$.

Clearly if the coercivity condition holds, then the operator \bar{Q}_T is strictly positive. For the other direction, suppose that $\inf_{h \in \mathcal{H}, \|h\|_{L^2(\bar{\rho}_T)}=1} \langle \bar{Q}_T h, h \rangle = 0$ for some compact subspace $\mathcal{H} \subset L^2(\bar{\rho}_T)$. Then there exists a sequence $\{h_n\}_{n=1}^\infty \subset \mathcal{H}$ with $\|h_n\|_{L^2(\bar{\rho}_T)} = 1$ such that $\langle \bar{Q}_T h_n, h_n \rangle \rightarrow 0$ as $n \rightarrow \infty$. Since the sequence is 100 bounded and \mathcal{H} is compact, there is an $h_* \in \mathcal{H}$ and a subsequence $h_{n_k} \rightarrow h_*$. This implies that $\|h_*\|_{L^2(\bar{\rho}_T)} = 1$ and $\langle \bar{Q}_T h_*, h_* \rangle = 0$, contradicting to the fact that \bar{Q}_T is strictly positive. ■

Similarly, we have the following proposition for the coercivity condition at a single time.

Proposition 2.4. *The system (1.1) with initial condition X^0 satisfies the coercivity conditions at time t if and only if the integral operator Q_t on $L^2(\rho_t)$ associated with the kernel*

$$K_t(r, s) := \frac{1}{\rho_t(r)\rho_t(s)} (rs)^{d-1} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p_t(r\xi, s\eta) d\xi d\eta. \quad (2.9)$$

is strictly positive.

Proof. Note that

$$\mathbb{E}[h(|\mathbf{r}_{12}^t|)h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}] = \int_0^\infty \int_0^\infty h(r)h(s)K_t(r, s)\rho_t(r)\rho_t(s)drds = \langle Q_t h, h \rangle$$

The proof is similar to the proof of Proposition 2.3. ■

105 With these operators, we consider the relation between the two types of coercivity conditions: whether it holds true on an interval if it holds true for each time in the interval. Equivalently, whether \bar{Q}_T on $L^2(\bar{\rho}_T)$ in Proposition 2.3 is positive if Q_t on $L^2(\rho_t)$ in Proposition 2.4 is positive for each time in $[0, T]$. Clearly, the question is subtle because these operators are defined on different spaces: $L^2(\rho_t)$ and $L^2(\bar{\rho}_T)$, and it requires additional constraints on ρ_t and $\bar{\rho}_T$, e.g. being equivalent. Instead of tackling operators on different
110 spaces, we provide a firm answer to the question for slightly modified operators, all on the space $L^2(\bar{\rho}_T)$, in the following proposition.

Proposition 2.5. *The integral operator \bar{Q}_T on $L^2(\bar{\rho}_T)$ associated with the kernel \bar{K}_T in (2.7) is strictly positive if $\{\tilde{Q}_t\}_{t \in [0, T]}$, the family of integral operators on $L^2(\bar{\rho}_T)$ associated with the kernels*

$$\tilde{K}_t(r, s) := \frac{1}{\bar{\rho}_T(r)\bar{\rho}_T(s)} (rs)^{d-1} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p_t(r\xi, s\eta) d\xi d\eta, \quad (2.10)$$

are positive for all t and strictly positive for some t .

Proof. Note that for any $h \in L^2(\bar{\rho}_T)$,

$$\langle \tilde{Q}_t h, h \rangle = \mathbb{E}[h(|\mathbf{r}_{12}^t|)h(|\mathbf{r}_{13}^t|) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}]$$

is continuous in $t \in [0, T]$ since the diffusion operator of system (2.1) is a continuous semigroup. Also, since the operator \tilde{Q}_t is non-negative for all t and positive for some t , so is $\langle \tilde{Q}_t h, h \rangle$. Noting that

$$\langle \bar{Q}_T h, h \rangle = \frac{1}{T} \int_0^T \langle \tilde{Q}_t h, h \rangle dt,$$

we have $\langle \bar{Q}_T h, h \rangle > 0$ if $h \neq 0$. ■

3. The case of linear systems

115 3.1. A macro-micro decomposition

Consider first the simplest case $\phi(r) \equiv \theta r$, or equivalently, $\Phi(r) = \frac{1}{2}\theta r^2$. The system (1.1) can be written as

$$d\mathbf{X}^t = -\theta \mathbf{A} \mathbf{X}^t dt + d\mathbf{B}^t, \quad (3.1)$$

where the matrix $\mathbf{A} \in \mathbb{R}^{Nd \times Nd}$ is given by (with I_d being the identity matrix on \mathbb{R}^d)

$$\mathbf{A} = \frac{1}{N} \begin{pmatrix} (N-1)I_d & -I_d & \cdots & -I_d \\ -I_d & (N-1)I_d & \cdots & -I_d \\ \vdots & \vdots & \ddots & \vdots \\ -I_d & -I_d & \cdots & (N-1)I_d \end{pmatrix}. \quad (3.2)$$

It is straightforward to compute that $\mathbf{A}^2 = \mathbf{A}$, and that the matrix \mathbf{A} has eigenvalue 1 of multiplicity $(N-1)d$ and eigenvalue 0 of multiplicity d . Note that the vector $\{\mathbf{x} = c(\mathbf{v}, \mathbf{v}, \dots, \mathbf{v})\}$ is a critical point of the deterministic system, for any constant $c \in \mathbb{R}$ and any vector $\mathbf{v} \in \mathbb{R}^d$.

By a macro-micro decomposition of the system as in [20, 21], the next lemma shows that the center of the particles moves like a Brownian motion, and the particles concentrates around the center with a Gaussian-like distribution.

Lemma 3.1. (i) The solution \mathbf{X}^t of Eq. (3.1) can be explicitly written as

$$\mathbf{X}^t = e^{-\theta t} \mathbf{A} \mathbf{X}^0 + \int_0^t e^{-\theta(t-s)} \mathbf{A} d\mathbf{B}^s + \mathbf{X}_c^t, \quad (3.3)$$

where $\mathbf{X}_c^t = (\mathbf{v}^t, \mathbf{v}^t, \dots, \mathbf{v}^t)'$ with $\mathbf{v}^t := \frac{1}{N} \sum_{i=1}^N \mathbf{X}_i^t = \frac{1}{N} \sum_{i=1}^N (\mathbf{X}_i^0 + \mathbf{B}_i^t)$.

(ii) Conditional on \mathbf{X}^0 , the centralized process $(\mathbf{Y}^t = \mathbf{X}^t - \mathbf{X}_c^t)$ is an Ornstein-Uhlenbeck process with marginal (in time) distribution $\mathcal{N}(e^{-\theta t} \mathbf{A} \mathbf{X}^0, \frac{1}{2\theta}(1 - e^{-\theta t}) \mathbf{A})$ for each t . In particular, if \mathbf{X}^0 is Gaussian and exchangeable with variance Σ , then for each t , \mathbf{Y}^t has a distribution $\mathcal{N}(\mathbf{0}, e^{-2\theta t} \mathbf{A} \Sigma \mathbf{A} + \frac{1}{2\theta}(1 - e^{-\theta t}) \mathbf{A})$.

Proof. Note first that $\mathbf{v}^t := \frac{1}{N} \sum_{i=1}^N \mathbf{X}_i^t = \frac{1}{N} \sum_{i=1}^N (\mathbf{X}_i^0 + \mathbf{B}_i^t)$ follows from the equation

$$d\mathbf{v}^t = \frac{1}{N} \sum_{i=1}^N d\mathbf{X}_i^t = \frac{1}{N} \sum_{i=1}^N d\mathbf{B}_i^t.$$

Next, note that $\mathbf{Y}^t = \mathbf{X}^t - \mathbf{X}_c^t = \mathbf{A} \mathbf{X}^t$ and

$$d\mathbf{Y}^t = \mathbf{A} d\mathbf{X}^t = -\theta \mathbf{A}^2 \mathbf{X}^t dt + \mathbf{A} d\mathbf{B}^t = -\theta \mathbf{Y}^t dt + \mathbf{A} d\mathbf{B}^t,$$

where we used $\mathbf{A}^2 = \mathbf{A}$ in the third equality. Therefore, (\mathbf{Y}^t) is an Ornstein-Uhlenbeck process

$$\mathbf{Y}^t = e^{-\theta t} \mathbf{Y}^0 + \int_0^t e^{-\theta(t-s)} \mathbf{A} d\mathbf{B}^s.$$

Therefore, conditional on \mathbf{X}^0 , with $\mathbf{Y}^0 = \mathbf{A} \mathbf{X}^0$ and $\mathbf{A}^2 = \mathbf{A}$, we have that the distribution of \mathbf{Y}^t is $\mathcal{N}(e^{-\theta t} \mathbf{A} \mathbf{X}^0, \frac{1}{2\theta}(1 - e^{-\theta t}) \mathbf{A})$ and that $\mathbf{X}^t = \mathbf{X}_c^t + \mathbf{Y}^t$ can be written as in (3.3).

If the initial distribution \mathbf{X}^0 is exchangeable, then $\mathbb{E}[\mathbf{Y}^0] = \mathbf{A} \mathbb{E}[\mathbf{X}^0] = \mathbf{0}$, because $\mathbb{E}[\mathbf{X}_i^0] = \mathbb{E}[\mathbf{X}_j^0]$ for any (i, j) . Thus, if \mathbf{X}^0 is Gaussian and exchangeable, then \mathbf{Y}^t is Gaussian with mean $\mathbf{0}$. The variance of \mathbf{Y}^t follows directly from the above integral representation. ■

We can also directly integrate Eq. (3.1) and write

$$\mathbf{X}^t = e^{-\theta \mathbf{A} t} \mathbf{X}^0 + \int_0^t e^{-\theta \mathbf{A}(t-s)} d\mathbf{B}^s.$$

But the distribution of \mathbf{X}^t conditional on \mathbf{X}^0 is $\mathcal{N}(e^{-\theta \mathbf{A} t} \mathbf{X}^0, \int_0^t e^{-2\mathbf{A}s} ds)$, in which the covariance is difficult to compute explicitly due to the singularity of the matrix \mathbf{A} . By introducing the centralized process \mathbf{Y}^t , though the distribution of \mathbf{Y}^t is degenerate with the covariance $\frac{1}{2\theta}(1 - e^{-\theta t}) \mathbf{A}$ being singular, we no longer need to compute $\int_0^t e^{-2\mathbf{A}s} ds$.

135 3.2. Coercivity condition for linear systems

Now we are ready to prove the coercivity conditions. We begin with two technical lemmas. Here denote by $\text{cov}(X, Y)$ the covariance of X and Y , with the convention that $\text{cov}(X) = \text{cov}(X, X)$.

140 **Lemma 3.2.** *Let (X, Y, Z) be exchangeable Gaussian random variables on \mathbb{R}^{3d} with covariance satisfying $\text{cov}(X) - \text{cov}(X, Y) = \lambda I_d$ for some $\lambda > 0$. Let $p^\lambda(u, v)$ denote the joint distribution of $(X - Y, X - Z)$ and $\rho^\lambda(r)$ denote the density function of $|X - Y|$. Then*

(i) $K^\lambda(r, s) : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}$ defined by

$$K^\lambda(r, s) := \frac{1}{\rho^\lambda(r)\rho^\lambda(s)}(rs)^{d-1} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p^\lambda(r\xi, s\eta) d\xi d\eta \quad (3.4)$$

is a nonnegative smooth function and in $L^2(\rho^\lambda \otimes \rho^\lambda)$.

(ii) The integral operator Q^λ associated with $K^\lambda(r, s)$ is strictly positive on $L^2(\rho^\lambda)$. Equivalently, for any $0 \neq h \in L^2(\mathbb{R}^+, \rho^\lambda)$,

$$\mathbb{E} \left[h(|X - Y|) h(|X - Z|) \frac{\langle X - Y, X - Z \rangle}{|X - Y||X - Z|} \right] > 0. \quad (3.5)$$

Proof. We first represent $K^\lambda(r, s)$ in terms a series of polynomials. By exchangeability, the random vector $(X - Y, X - Z)$ is centered Gaussian with covariance matrix $\lambda \begin{pmatrix} 2I_d & I_d \\ I_d & 2I_d \end{pmatrix}$, whose inverse is $\frac{1}{3\lambda} \begin{pmatrix} 2I_d & -I_d \\ -I_d & 2I_d \end{pmatrix}$. Thus, the joint distribution is $p^\lambda(u, v) = (2\sqrt{3}\pi\lambda)^{-d} e^{-\frac{1}{3\lambda}(|u|^2 + |v|^2 - \langle u, v \rangle)}$. Combining with the fact that

$$\rho^\lambda(r) = \frac{1}{C_\lambda} r^{d-1} e^{-\frac{r^2}{4\lambda}}$$

with $C_\lambda = \frac{1}{2}(4\lambda)^{\frac{d}{2}}\Gamma(\frac{d}{2})$ and that the surface area of the unit sphere is $|S^{d-1}| = \frac{2\pi^{d/2}}{\Gamma(\frac{d}{2})}$, the integral kernel in (3.4) can be written as

$$K^\lambda(r, s) = C_d e^{-\frac{1}{12\lambda}(r^2 + s^2)} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle e^{c_\lambda r s \langle \xi, \eta \rangle} \frac{d\xi d\eta}{|S^{d-1}|^2}$$

with $C_d = (\frac{\sqrt{3}}{2})^{-d}$ and $c_\lambda = \frac{1}{3\lambda}$. Here when $d = 1$, the above spherical measure on $S^0 = \{-1, 1\}$ is interpreted as $\mathbb{P}(\xi = 1) = \mathbb{P}(\xi = -1) = \frac{1}{2}$, or equivalently, $\int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle e^{\frac{1}{3\lambda}(rs\langle \xi, \eta \rangle)} \frac{d\xi d\eta}{|S^{d-1}|^2} = \frac{1}{2}(e^{c_\lambda r s} - e^{-c_\lambda r s})$. By Taylor expansion

$$\langle \xi, \eta \rangle e^{c_\lambda r s \langle \xi, \eta \rangle} = \sum_{k=1}^{\infty} \frac{1}{(k-1)!} c_\lambda^{k-1} (rs)^{k-1} \langle \xi, \eta \rangle^k,$$

and the fact that

$$b_k = \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle^k \frac{d\xi d\eta}{|S^{d-1}|^2} \begin{cases} = 0, & \text{for odd } k, \\ \in (0, 1), & \text{for even } k, \end{cases}$$

we have

$$K^\lambda(r, s) = C_d e^{-\frac{1}{12\lambda}(r^2 + s^2)} \sum_{k=0}^{\infty} \frac{1}{k!} c_\lambda^k b_{k+1} (rs)^k = C_d e^{-\frac{1}{12\lambda}(r^2 + s^2)} \sum_{k=1, k \text{ odd}}^{\infty} \frac{1}{k!} c_\lambda^k b_{k+1} (rs)^{k-1}$$

Thus, $K^\lambda(r, s)$ is non-negative smooth and in $L^2(\rho^\lambda \times \rho^\lambda)$.

To prove (ii), since Q^λ is the integral operator associated with $K^\lambda(r, s)$ on $L^2(\mathbb{R}^+, \rho^\lambda)$, we have, for any

$h \in L^2(\mathbb{R}^+, \rho^\lambda)$,

$$\begin{aligned} \langle Q^\lambda h, h \rangle_{L^2(\rho^\lambda)} &= \int_0^\infty h(r)h(s)K^\lambda(r, s)\rho^\lambda(r)\rho^\lambda(s)drds \\ &= C_d \sum_{k=1, k \text{ odd}}^\infty \frac{1}{k!} c_\lambda^k b_{k+1} \left(\int_0^\infty h(r)r^{k-1}e^{-\frac{1}{12\lambda}r^2}\rho^\lambda(r)dr \right)^2 \geq 0. \end{aligned}$$

Note that

$$\int_0^\infty h(r)r^{k-1}e^{-\frac{1}{12\lambda}r^2}\rho^\lambda(r)dr = C_\lambda^{-1} \int_0^\infty h(r)r^{k+d-2}e^{-\frac{1}{3\lambda}r^2}dr$$

By Lemma 5.9, a variation of the Müntz Theorem, the space $\text{span}\{1, r^2, r^4, r^6, \dots\}$ is dense in $L^2(r^{d-1}e^{-\frac{1}{3\lambda}r^2})$. Thus, $\langle Q^\lambda h, h \rangle_{L^2(\rho^\lambda)} = 0$ only if $h \equiv 0$. Therefore, Q^λ is strictly positive. ■

Lemma 3.3. Let (X_t, Y_t, Z_t) be a family of exchangeable Gaussian random variables on \mathbb{R}^{3d} with covariance satisfying $\text{cov}(X) - \text{cov}(X, Y) = \lambda(t)I_d$ with $\lambda(t) = e^{-2\theta t}\lambda_0 + \frac{1}{2\theta}(1 - e^{-\theta t})$ for $t \in [0, T]$, $\theta > 0$ and $\lambda_0 > 0$. Let $p^t(u, v)$ denote the joint distribution of $(X_t - Y_t, X_t - Z_t)$, $\rho^t(r)$ denote the density function of $|X_t - Y_t|$, and let

$$\bar{\rho}(r) := \frac{1}{T} \int_0^T \rho^t(r)dt. \quad (3.6)$$

$$\tilde{K}^t(r, s) := \frac{1}{\bar{\rho}(r)\bar{\rho}(s)}(rs)^{d-1} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p^t(r\xi, s\eta) d\xi d\eta. \quad (3.7)$$

145 Then the integral operators $\{\tilde{Q}^t\}_{t \in [0, T]}$ on $L^2(\bar{\rho})$ associated with \tilde{K}^t is uniformly bounded, continuous in t , and strictly positive for each t .

Proof. The proof is similar to the proof of Lemma 3.2. we represent $\tilde{K}^t(r, s)$ in a series of polynomials and prove that the operator \tilde{Q}^t is positive by the Müntz Theorem. First, note that

$$\tilde{K}^t(r, s) = C_{d, \lambda(t)} \frac{1}{\bar{\rho}(r)\bar{\rho}(s)} (rs)^{d-1} e^{-c_\lambda(r^2+s^2)} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle e^{c_\lambda r s \langle \xi, \eta \rangle} \frac{d\xi d\eta}{|S^{d-1}|^2}$$

with $C_{d, \lambda(t)} > 0$ and $c_\lambda = \frac{1}{3\lambda(t)}$. Then, for any $h \in L^2(\mathbb{R}^+, \bar{\rho})$,

$$\begin{aligned} \langle \tilde{Q}^t h, h \rangle_{L^2(\bar{\rho})} &= \int_0^\infty h(r)h(s)\tilde{K}^t(r, s)\bar{\rho}(r)\bar{\rho}(s)drds \\ &= C_{d, \lambda(t)} \sum_{k=1, k \text{ odd}}^\infty \frac{1}{k!} c_\lambda^k b_{k+1} \left(\int_0^\infty h(r)r^{k+d-2}e^{-\frac{1}{3\lambda(t)}r^2}dr \right)^2 \geq 0. \end{aligned}$$

Then it follows from Lemma 5.9 that the space $\text{span}\{1, r^2, r^4, r^6, \dots\}$ is dense in $L^2(r^{d-1}e^{-\frac{1}{3\lambda(t)}r^2})$. Thus, $\langle \tilde{Q}^t h, h \rangle_{L^2(\bar{\rho})} = 0$ only if $h \equiv 0$. Therefore, \tilde{Q}^t is strictly positive. ■

150 **Theorem 3.4.** Suppose the linear system (3.1) starts with an initial distribution of $(\mathbf{X}_1^0, \dots, \mathbf{X}_N^0)$ that is exchangeable Gaussian with covariance satisfying $\text{cov}(\mathbf{X}_i^0) - \text{cov}(\mathbf{X}_i^0, \mathbf{X}_j^0) = \lambda_0 I_d$ with $\lambda_0 > 0$ for all $1 \leq i < j \leq N$. Then, (i) the coercivity condition holds true at each time $t \geq 0$ in the sense of Definition 2.2; (ii) the coercivity condition also holds true on $[0, T]$ in the sense of Definition 2.1

Proof. Let $\mathbf{Y}^t = \mathbf{X}^t - \mathbf{X}_c^t$. Note that

$$\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t = \mathbf{Y}_i^t - \mathbf{Y}_j^t.$$

Thus, the coercivity conditions for the process (\mathbf{X}^t) is equivalent to those for the process (\mathbf{Y}^t) .

By Lemma 3.1 $(\mathbf{Y}_1^t, \dots, \mathbf{Y}_N^t)$ is exchangeable Gaussian with covariance satisfying $\text{cov}(\mathbf{Y}_i^t) - \text{cov}(\mathbf{Y}_i^t, \mathbf{Y}_j^t) = [e^{-2\theta t}\lambda_0 + \frac{1}{2\theta}(1 - e^{-\theta t})] I_d$. In particular, the vector $(\mathbf{Y}_1^t, \mathbf{Y}_2^t, \mathbf{Y}_3^t)$ is exchangeable Gaussian with $\text{cov}(\mathbf{Y}_i^t) -$

$\text{cov}(\mathbf{Y}_i^t, \mathbf{Y}_j^t) = (e^{-2\theta t} + \frac{1}{2\theta}(1 - e^{-\theta t})) I_d$. By Lemma 3.2, the integral operator associated with the kernel (2.9) is strictly positive on $L^2(\rho_t)$. Part (i) then follows from Proposition 2.4.

Part (ii) follows from Proposition 2.5 and Lemma 3.3 because $(\mathbf{X}_1^t, \mathbf{X}_2^t, \mathbf{X}_3^t)$ are exchangeable Gaussian satisfying the covariance condition with $\lambda(t) = e^{-2\theta t}\lambda_0 + \frac{1}{2\theta}(1 - e^{-\theta t})$ for $t \in [0, T]$. ■

160 **Remark 3.5.** When the system is deterministic, i.e. there is no stochastic force, the coercivity conditions hold true when the initial distribution is exchangeable Gaussian with $\text{cov}(\mathbf{X}_i^0) - \text{cov}(\mathbf{X}_i^0, \mathbf{X}_j^0) = \lambda_0 I_d$. In this case, we simply have $\mathbf{X}^t = e^{-\theta t} \mathbf{A} \mathbf{X}^0 + \mathbf{X}_c^t$ and $\mathbf{Y}^t = e^{-\theta t} \mathbf{A} \mathbf{X}^0$. Then the vector $(\mathbf{Y}_1^t, \mathbf{Y}_2^t, \mathbf{Y}_3^t)$ is exchangeable Gaussian with $\text{cov}(\mathbf{Y}_i^t) - \text{cov}(\mathbf{Y}_i^t, \mathbf{Y}_j^t) = e^{-2\theta t} \lambda_0 I_d$. Again coercivity follows from Lemmas 3.2 3.3. In particular, this holds when the initial distribution is standard Gaussian, in which case $\lambda_0 = 1$.

165 3.3. Coercivity condition for non-radial interaction functions

The covariance condition $\text{cov}(\mathbf{X}_i^0) - \text{cov}(\mathbf{X}_i^0, \mathbf{X}_j^0) = \lambda_0 I_d$ in Theorem 3.4 is necessary for the above proof, due to the need of series representation of the radial integral kernel K_t . This condition can be removed when we prove the coercivity condition based on a series representation of the corresponding non-radial integral kernel. More importantly, we show in this section that identifiability holds true for interaction functions 170 that are non-radial, depending on the pairwise differences between positions.

It is straightforward to see from Section 2.1 that for non-radial interaction functions, the function space of learning is $L^2(\mathbb{R}^d, \bar{\rho}_T)$ or $L^2(\mathbb{R}^d, \rho_t)$ with

$$\bar{\rho}_T(\mathbf{r}) = \frac{1}{T} \int_0^T \rho_t(\mathbf{r}) dt, \quad \text{with } \rho_t(\mathbf{r}) = \mathbb{E}[\delta(\mathbf{X}_i^t - \mathbf{X}_j^t - \mathbf{r})]. \quad (3.8)$$

Correspondingly, the coercivity condition is on $L^2(\mathbb{R}^d, \bar{\rho}_T)$ or $L^2(\mathbb{R}^d, \rho_t)$.

Definition 3.6 (Coercivity condition for non-radial functions). The dynamical system (1.1) on $[0, T]$ with initial condition \mathbf{X}^0 is said to satisfy the coercivity condition on a compact subspace $\mathcal{H} \subset L^2(\mathbb{R}^d, \bar{\rho}_T)$, with $\bar{\rho}_T$ defined in (3.8), if

$$c_{\mathcal{H}, T} := \inf_{h \in \mathcal{H}, \|h\|_{L^2(\bar{\rho}_T)} = 1} \frac{1}{T} \int_0^T \mathbb{E}[h(\mathbf{r}_{12}^t) h(\mathbf{r}_{13}^t) \frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t| |\mathbf{r}_{13}^t|}] dt > 0, \quad (3.9)$$

where $\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t$. If the coercivity condition holds true on every compact subspace $\mathcal{H} \subset L^2(\mathbb{R}^d, \bar{\rho}_T)$, we say the system satisfies the coercivity condition. Similarly, we can define the coercivity condition at a single time t on $L^2(\mathbb{R}^d, \rho_t)$.

175 Propositions 2.3 and 2.4 can be directly generalized to the non-radial version. So we may prove the coercivity condition by showing that the corresponding integral operator is strictly positive. The proof will be based on a series representation of the non-radial integral kernel. First, we need a key lemma showing that polynomials are dense on some weighted L^2 spaces.

Lemma 3.7. [22] Lemma 1.1] Let μ be a measure on \mathbb{R}^d satisfying

$$\int e^{c|x|} d\mu(x) < \infty$$

for some $c > 0$, where $|x| = \sum_{j=1}^d |x_j|$. Then the polynomials are dense in $L^2(\mu)$.

Proposition 3.8. Let X, Y, Z be exchangeable Gaussian random variables on \mathbb{R}^d with a non-degenerate distribution. Let $p(u, v)$ denote the non-degenerate joint density of $(X - Y, X - Z)$ and let $\rho(u)$ denote the density of $X - Y$. Then the integral operator Q associated with the kernel

$$K(u, v) := \frac{1}{\rho(u)\rho(v)} \langle u, v \rangle p(u, v) \quad (3.10)$$

180 is strictly positive on $L^2(\mathbb{R}^d, \rho)$.

Proof. Since $h \in L^2(\mathbb{R}^d, \rho)$ and X, Y, Z are exchangeable, we have by Cauchy-Schwarz

$$|\langle Qh, g \rangle| = \left| \mathbb{E}[h(X-Z)g(X-Z) \frac{\langle X-Y, X-Z \rangle}{\|X-Y\|\|X-Z\|}] \right| \leq \|h\|_{L^2(\rho)} \|g\|_{L^2(\rho)}$$

so Q is a bounded operator on $L^2(\rho)$. To show that Q is strictly positive, we need to prove (i) $\langle Qh, h \rangle \geq 0$ for any $h \in L^2(\rho)$, and (ii) $\langle Qh, h \rangle = 0 \Rightarrow h = 0$ in $L^2(\rho)$.

Proof of (i): to show that for all $h \in L^2(\rho)$,

$$\langle Qh, h \rangle = \iint h(u)h(v) \frac{\langle u, v \rangle}{|u||v|} p(u, v) du dv \geq 0, \quad (3.11)$$

by Theorem 5.2 it suffices to show $p(u, v)$ is positive definite. Suppose that $X, Y, Z \sim N(\mu, \Sigma)$ with Σ invertible since the distribution is non-degenerate. Decompose $\Sigma^{-1} = LL^T$. Then $L(X-\mu), L(Y-\mu), L(Z-\mu) \sim N(0, I)$. Denote them by $\tilde{X}, \tilde{Y}, \tilde{Z}$, respectively. By Theorem 5.2 it suffices to show the density of $(\tilde{X} - \tilde{Y}, \tilde{X} - \tilde{Z})$ is positive definite. Since $\tilde{X}, \tilde{Y}, \tilde{Z}$ are exchangeable, $\text{cov}(\tilde{X}, \tilde{Y}) = \text{cov}(\tilde{X}, \tilde{Z}) = \text{cov}(\tilde{Y}, \tilde{Z})$. Let $\Theta = \text{cov}(\tilde{X}, \tilde{Y}) = \mathbb{E}[\tilde{X}\tilde{Y}^T]$. Since Θ is real symmetric, it can be diagonalizable by a real orthogonal matrix P . Write $P\Theta P^T = \text{diag}(\lambda_1, \dots, \lambda_d)$, where $-1 \leq \lambda_i < 1$ by the non-degeneracy assumption. Denote $P\tilde{X}, P\tilde{Y}, P\tilde{Z}$ by X', Y', Z' respectively. By Theorem 5.2 again, it suffices to show that the density $q(u, v)$ of $(X' - Y', X' - Z')$ is positive definite. Then the covariance matrix

$$\text{cov}(X' - Y', X' - Z') = \begin{bmatrix} 2I - 2\Theta & I - \Theta \\ I - \Theta & 2I - 2\Theta \end{bmatrix},$$

which has the inverse (by the non-degeneracy assumption)

$$\text{cov}(X' - Y', X' - Z')^{-1} = \frac{1}{3} \begin{bmatrix} 2\Lambda & -\Lambda \\ -\Lambda & 2\Lambda \end{bmatrix}$$

where $\Lambda := \text{diag}(\frac{1}{1-\lambda_1}, \dots, \frac{1}{1-\lambda_d})$. Thus for some normalizing constant $C_d > 0$, $q(u, v)$ is equal to

$$\begin{aligned} & C_d \exp(-\frac{1}{2}(u, v) \text{cov}(X' - Y', X' - Z')^{-1}(u, v)^T) \\ &= C_d \exp(\frac{1}{3}(\sum_{i=1}^d \frac{u_i^2}{\lambda_i - 1} + \sum_{i=1}^d \frac{v_i^2}{\lambda_i - 1} + \sum_{i=1}^d \frac{u_i v_i}{1 - \lambda_i})). \end{aligned}$$

By Theorem 5.2 and the fact that $-1 \leq \lambda_i < 1$, $q(u, v)$ is positive definite. Then (i) is proved.

Proof of (ii): Let $h \in L^2(\rho)$ satisfy $\langle Qh, h \rangle = 0$. We need to prove that $h = 0$. Denote $a_i := \frac{1}{1-\lambda_i} \geq \frac{1}{2}$,

$$b(u) := \exp(-\frac{1}{3} \sum_{i=1}^d a_i u_i^2),$$

$$f(u, v) := \exp(\frac{1}{3} \sum_{i=1}^d a_i u_i v_i).$$

By the linear transform $X \mapsto PL(X - \mu)$, we may rewrite (3.11) as

$$\langle Qh, h \rangle = C_d (\det L)^2 \sum_{j=1}^d \iint g_j(u) g_j(v) f(u, v) du dv,$$

where $g_j(u) = b(u) h((PL)^{-1}u) \frac{((PL)^{-1}u)_j}{|(PL)^{-1}u|}$. Note that by Taylor expansion

$$f(u, v) = \sum_{k=0}^{\infty} \frac{1}{k! 3^k} (\sum_{i=1}^d a_i u_i v_i)^k = \sum_{k=0}^{\infty} \sum_{i_1 + \dots + i_d = k} C_{k, i_1, \dots, i_d} (u_1 v_1)^{i_1} \dots (u_d v_d)^{i_d},$$

which is a linear combination of all the d -variable monomials $u_1^{i_1} \cdots u_d^{i_d}$ and all coefficients are positive. Thus by Fubini

$$\langle Qh, h \rangle = C_d (\det L)^2 \sum_j \sum_{k, i_1, \dots, i_d} C_{k, i_1, \dots, i_d} \left(\int g_j(u) u_1^{i_1} \cdots u_d^{i_d} du \right)^2 = 0 \quad (3.12)$$

which implies each term must be zero

$$\int g_j(u) u_1^{i_1} \cdots u_n^{i_n} du = 0, \text{ for any integers } i_1, \dots, i_d \geq 0.$$

Then for any polynomial $\phi(u)$ we have

$$\int g_j(u) \phi(u) du = 0.$$

Note that the marginal density of $(X' - Y', X' - Z')$ is equal to

$$q(u) := \int q(u, v) dv = C'_d \exp\left(-\frac{1}{4} \sum_{i=1}^d a_i u_i^2\right)$$

for some normalizing constant $C'_d > 0$. Then $h(u) \in L^2(\mathbb{R}^d, \rho)$ implies $h((PL)^{-1}u) \in L^2(\mathbb{R}^d, q)$.

Let $\tilde{g}_j(u) := \exp(-\frac{1}{12} \sum_{i=1}^d a_i u_i^2) h((PL)^{-1}u) \frac{((PL)^{-1}u)_j}{|(PL)^{-1}u|}$. Since $|\tilde{g}_j(u)| \leq |h((PL)^{-1}u)|$, we get $\tilde{g}_j(u) \in L^2(\mathbb{R}^d, q)$. Recall that for any polynomial $\phi(u)$ we have

$$\int g_j(u) \phi(u) du = \int \tilde{g}_j(u) \phi(u) d\mu(u) = 0,$$

185 where $d\mu(u) := q(u)du$. Clearly, the measure μ satisfies the condition of Lemma 3.7. Then the polynomials are dense in $L^2(\mathbb{R}^d, q)$, therefore, $\tilde{g}_j = 0$ and hence $h = 0$ in $L^2(\mathbb{R}^d, \rho)$. ■

Theorem 3.9. Suppose the linear system (3.1) starts with an initial distribution of $(\mathbf{X}_1^0, \dots, \mathbf{X}_N^0)$ that is non-degenerate exchangeable Gaussian. Then the coercivity condition holds true at each time $t \geq 0$, as well as on $[0, T]$, in the sense of Definition 3.6.

Proof. Let $\mathbf{Y}^t = \mathbf{X}^t - \mathbf{X}_c^t$. Note that

$$\mathbf{r}_{ij}^t = \mathbf{X}_i^t - \mathbf{X}_j^t = \mathbf{Y}_i^t - \mathbf{Y}_j^t.$$

190 Thus, the coercivity conditions for the process (\mathbf{X}^t) are equivalent to those for the process (\mathbf{Y}^t) .

By Lemma 3.1 $(\mathbf{Y}_1^t, \dots, \mathbf{Y}_N^t)$ is exchangeable Gaussian. In particular, the vector $(\mathbf{Y}_1^t, \mathbf{Y}_2^t, \mathbf{Y}_3^t)$ is exchangeable Gaussian. By Proposition 3.8, the integral operator Q_t associated with the kernel

$$K_t(u, v) := \frac{1}{\rho_t(u)\rho_t(v)} \langle u, v \rangle p_t(u, v) \quad (3.13)$$

is strictly positive on $L^2(\rho_t)$. Then it follows from the non-radial version of Proposition 2.4 that the coercivity condition holds true for each time t .

The coercivity on $[0, T]$ follows from the non-radial version of Proposition 2.3 immediately by using a similar argument to show the integral operator \bar{Q}_T associated with the kernel

$$\bar{K}_T(u, v) := \frac{1}{\bar{\rho}_T(u)\bar{\rho}_T(v)} \langle u, v \rangle \int_0^T p_t(u, v) dt \quad (3.14)$$

is strictly positive on $L^2(\bar{\rho}_T)$, since the proof of Proposition 3.8 still works if we replace Q by \bar{Q}_T , $K(u, v)$ by $\bar{K}_T(u, v)$, ρ by $\bar{\rho}_T$, $p(u, v)$ by $\frac{1}{T} \int_0^T p_t(u, v) dt$, $q(u, v)$ by $\frac{1}{T} \int_0^T q_t(u, v) dt$, etc. In particular, (3.12) is replaced by

$$\langle \bar{Q}_T h, h \rangle = \frac{1}{T} \int_0^T C_d(t) (\det L(t))^2 \sum_j \sum_{k, i_1, \dots, i_n} C_{k, i_1, \dots, i_n}(t) \left(\int g_j(t, u) u_1^{i_1} \cdots u_n^{i_n} du \right)^2 dt = 0$$

where the positive coefficients C_d , $\det L$, and C_{k,i_1,\dots,i_n} depend on t . It still implies $g_j = 0$, and then $h = 0$. ■

4. Nonlinear systems with three particles

We consider a class of nonlinear systems with $N = 3$ and with stationary distribution — in this case, if the coercivity condition holds true on a time instance as in Definition 2.2, then it also holds on any time interval (see Definition 2.1).

When $N = 3$, the stationary distribution of $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$, as we show below, can be computed analytically from a closed differential equation of these two variables. We then prove the coercivity condition based on the analytical form of the stationary distribution. When $N > 3$, there is no closed system for this process, and the computation of the distribution of $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$ requires marginalization, which makes the analytical form intractable.

We introduce a “comparison to Gaussian kernels” technique, which makes extensive use of positive definite kernels, to prove the coercivity condition, see Section 4.2. This technique allows us to consider a large class of interaction potentials that lead to positive definite stationary distributions. These potentials include $\Phi(r) = r^{2\beta}$ and $\Phi(r) = \Phi_0(r) + cr^{2\beta}$, where $\beta \in [1/2, 1]$ and $\Phi_0(r)$ is a smooth positive definite function.

4.1. Stationary distribution for pairwise differences

Global solutions exist for the gradient system (2.1) with potentials $\Phi(r) = r^{2\beta}$ or $\Phi(r) = \Phi_0(r) + cr^{2\beta}$, if $\beta \in [1/2, 1]$ and $\Phi_0(r)$ is smooth, because these potentials lead to continuous drift terms. When $\beta < 1/2$, these potentials lead to singular drifts, and we refer to [23, 17] for further study on the existence of weak and strong solutions.

We show first that the process of pairwise differences $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$ admits a stationary distribution, though the whole system of the particles does not.

Proposition 4.1. *Suppose that $\Phi \in C^1(\mathbb{R}^+, \mathbb{R}^+)$ and $Z = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{-H(u,v)} du dv < \infty$ for*

$$H(u, v) = \frac{1}{3}[\Phi(|u|) + \Phi(|v|) + \Phi(|u - v|)].$$

Then the process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t) = (\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$ admits an invariant probability density

$$p(u, v) = \frac{1}{Z} e^{-2H(u,v)}. \quad (4.1)$$

Proof. Note that

$$\begin{cases} d\mathbf{r}_{12}^t &= F(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)dt + (d\mathbf{B}_1^t - d\mathbf{B}_2^t), \\ d\mathbf{r}_{13}^t &= F(\mathbf{r}_{13}^t, \mathbf{r}_{12}^t)dt + (d\mathbf{B}_1^t - d\mathbf{B}_3^t), \end{cases} \quad (4.2)$$

where the function $F : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ is given by

$$F(u, v) = -\frac{1}{3}[2\phi(|u|)u + \phi(|v|)v + \phi(|u - v|)(u - v)],$$

where $\phi(r) = \Phi'(r)$.

The diffusion $\begin{pmatrix} d\mathbf{B}_1^t - d\mathbf{B}_2^t \\ d\mathbf{B}_1^t - d\mathbf{B}_3^t \end{pmatrix}$ has a non-degenerate covariance $\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$. One can then verify directly that the distribution $p(u, v)$ is a stationary solution to the backward Kolmogorov equation of (4.2). Alternatively, for simpler computation, we show that the system (4.2) is a linear transformation of a gradient system with homogeneous diffusion, which shares the same invariant measure. Let $A = \sqrt{2} \begin{pmatrix} 1 & 0 \\ 1/2 & \sqrt{3}/2 \end{pmatrix}$, which satisfies

$AA^T = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$. Then the process

$$\begin{pmatrix} \mathbf{Y}_1^t \\ \mathbf{Y}_2^t \end{pmatrix} = A^{-1} \begin{pmatrix} \mathbf{r}_{12}^t \\ \mathbf{r}_{13}^t \end{pmatrix}$$

is a weak solution to the system

$$d \begin{pmatrix} \mathbf{Y}_1^t \\ \mathbf{Y}_2^t \end{pmatrix} = A^{-1} \begin{pmatrix} F(\mathbf{Y}_1^t, \frac{\sqrt{2}}{2}\mathbf{Y}_1^t + \frac{\sqrt{6}}{2}\mathbf{Y}_2^t) \\ F(\frac{\sqrt{2}}{2}\mathbf{Y}_1^t + \frac{\sqrt{6}}{2}\mathbf{Y}_2^t, \mathbf{Y}_1^t) \end{pmatrix} dt + \begin{pmatrix} d\tilde{\mathbf{B}}_1^t \\ d\tilde{\mathbf{B}}_2^t \end{pmatrix}, \quad (4.3)$$

where $(\tilde{\mathbf{B}}_1^t, \tilde{\mathbf{B}}_2^t)$ is a standard Brownian motion on \mathbb{R}^{2d} . Notice that $H(u, v) = H(v, u)$ and

$$A^{-1} \begin{pmatrix} F(\sqrt{2}u, \frac{\sqrt{2}}{2}u + \frac{\sqrt{6}}{2}v) \\ F(\frac{\sqrt{2}}{2}u + \frac{\sqrt{6}}{2}v, \sqrt{2}u) \end{pmatrix} = \begin{pmatrix} \nabla_u [H(\sqrt{2}u, \frac{\sqrt{2}}{2}u + \frac{\sqrt{6}}{2}v)] \\ \nabla_v [H(\frac{\sqrt{2}}{2}u + \frac{\sqrt{6}}{2}v, \sqrt{2}u)] \end{pmatrix}.$$

Then, it follows from Lemma 5.10 that $p_{\mathbf{Y}}(\mathbf{y}_1, \mathbf{y}_2) \propto e^{-2H(\mathbf{y}_1, \frac{\sqrt{2}}{2}\mathbf{y}_1 + \frac{\sqrt{6}}{2}\mathbf{y}_2)}$ is an invariant density for the system (4.3). Therefore, the process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$ admits $p(u, v)$ as an invariant density. ■

Remark 4.2. Similarly, one can prove that the process $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t, \dots, \mathbf{X}_1^t - \mathbf{X}_N^t)$ admits a stationary density on $\mathbb{R}^{(N-1)d}$. In essence, we decompose the system into a reference particle and the relative positions of other particle to the reference particle. This is similar to the macro-micro decomposition of the system in [20, 24, 25, 27]. But the above transformation leads to a gradient system with an additive white noise. This simplifies the proof of the stationary distribution. Furthermore, the distribution of relative position $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$ is the information necessary for the study of the weak solution of the system.

Remark 4.3. Our current proofs for coercivity condition makes use of the explicit form of the joint distribution of $(\mathbf{X}_1^t - \mathbf{X}_2^t, \mathbf{X}_1^t - \mathbf{X}_3^t)$. When there are more than three particles, such an explicit distribution is no longer available due to the need of marginalization, except the Gaussian case. We expect to develop new techniques to make further use of the exchangeability to avoid marginalization.

4.2. Interaction potentials in form of $\Phi(r) = r^{2\beta}$

We develop in this section a “comparison to Gaussian kernels” technique to prove that the coercivity condition holds true for systems with interaction potential $\Phi(r) = r^{2\beta}$ for $0 < \beta \leq 1$ and starting from an initial condition such that the pairwise difference has the stationary distribution.

This technique is based on that the stationary distribution of the stationary distribution $p(u, v)$ defined in (4.1) is positive definite, which we prove in the next lemma.

Lemma 4.4. Assume $\Phi(r) = r^{2\beta}$.

1. If $0 < \beta \leq 1$, then $e^{-\Phi(|u-v|)}$ is a positive definite kernel, so is $p(u, v)$ defined in (4.1).
2. If $\beta > 1$, then $p(u, v)$ defined in (4.1) is not positive definite.

Proof. This is a generalization of Corollary 3.3.3 of [26] to the high-dimensional case. Note that $p(u, v)$ is positive definite if and only if $e^{-\Phi(|u-v|)}$ is positive definite. The kernel $|u - v|^2$ for $u, v \in \mathbb{R}^d$ is a negative definite kernel, because for any $c_1, \dots, c_n \in \mathbb{R}$, and $\sum_{i=1}^n c_i = 0$,

$$\begin{aligned} \sum_{i,j=1}^n c_i c_j |u_i - u_j|^2 &= \left[\sum_{i=1}^n c_i \right] \left[\sum_{j=1}^n c_j |u_j|^2 \right] + \left[\sum_{j=1}^n c_j \right] \left[\sum_{i=1}^n c_i |u_i|^2 \right] - \left| \sum_{i=1}^n c_i u_i \right|^2 \\ &= - \left| \sum_{i=1}^n c_i u_i \right|^2 \leq 0. \end{aligned}$$

By Theorem 5.6, $|u - v|^{2\beta}$ is also a negative definite kernel for any $0 < \beta \leq 1$. By Theorem 5.5, we obtain that $e^{-|u-v|^{2\beta}}$ is positive definite, then Part (1) follows.

Now we prove Part (2). Suppose now that for some $\beta > 1$, $p(u, v)$ is a positive definite kernel. Then for any $t > 0$, $x_1, \dots, x_n \in \mathbb{R}^d$ and $c_1, \dots, c_n \in \mathbb{R}$, we have

$$\sum_{j,k=1}^n c_j c_k e^{-t|x_j - x_k|^{2\beta}} = \sum_{j,k=1}^n c_j c_k e^{-\left| t^{\frac{1}{2\beta}} x_j - t^{\frac{1}{2\beta}} x_k \right|^{2\beta}} \geq 0$$

245 By Theorem 5.5, the kernel $|u - v|^{2\beta}$ is negative definite, and by Theorem 5.7, $|u - v|^\beta$ is a metric on \mathbb{R} . Let $\mathbf{0} = (0, \dots, 0) \in \mathbb{R}^d$, $\mathbf{1} = (1, \dots, 1) \in \mathbb{R}^d$ and $\mathbf{2} = (2, \dots, 2) \in \mathbb{R}^d$. Note that

$$|\mathbf{0} - \mathbf{1}|^\beta = d^{\frac{\beta}{2}}, \quad |\mathbf{0} - \mathbf{2}|^\beta = 2^\beta d^{\frac{\beta}{2}} > 2|\mathbf{0} - \mathbf{1}|^\beta$$

when $\beta > 1$. The contradiction to the triangle inequality implies Part (2). ■

Recall that the coercivity condition depending only on the distribution of the process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$. When the process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$ is stationary, the coercivity condition at a time instance in Definition 2.2 is equivalent to that of Definition 2.1.

250 Following proposition 2.3, the coercivity condition is equivalent to the positiveness of the integral operator associated with $K(r, s) : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}$ defined by

$$K(r, s) := \frac{1}{\rho(r)\rho(s)} (rs)^{d-1} \int_{S^{d-1}} \int_{S^{d-1}} \langle \xi, \eta \rangle p(r\xi, s\eta) d\xi d\eta, \quad (4.4)$$

where $p(u, v)$ is the stationary density defined in (4.1), and ρ denotes the density of $|\mathbf{r}_{12}^t|$. For the case $\beta = 1$ in the previous section, we witnessed that the Gaussian distribution neatly ensures strict positiveness of the integral operator through Taylor expansion of $\langle u, v \rangle e^{c\langle u, v \rangle}$. However, when $\beta \neq 1$, such a “quadratic structure” is no longer available. We introduce a new technique, which bounds the kernel by another positive definite kernel from below and combines the Gamma integral representation of the power function, to uncover such a quadratic structure.

Lemma 4.5. *Let $\Phi_i : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ be positive definite kernels for $i = 1, 2$. Then*

$$\begin{aligned} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u)h(v)\Phi_1(u, v)e^{\Phi_2(u, v)}dudv &\geq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u)h(v)\Phi_1(u, v)dudv, \\ \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u)h(v)\Phi_1(u, v)e^{\Phi_2(u, v)}dudv &\geq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(u)h(v)\Phi_1(u, v)\Phi_2(u, v)dudv, \end{aligned}$$

as long as the integrals exist.

Proof. By Theorem 5.2, $\Phi_2(u, v)^n \Phi_1(u, v)$ is positive definite for each integer $n \geq 0$. Then the inequalities follow from the Taylor expansion of $e^{\Phi_2(u, v)}$. ■

Proposition 4.6. *Let $\beta \in (0, 1]$ and $p(u, v)$ be a probability density function defined in (4.1) with $\Phi(r) = r^{2\beta}$, i.e. $p(u, v) = \frac{1}{Z} e^{-\frac{2}{3}(|u|^{2\beta} + |v|^{2\beta} + |u - v|^{2\beta})}$. Let $\rho(r)$ be the probability density function of $|U|$ with (U, V) having a joint distribution $p(u, v)$. Then,*

$$I = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(|u|)h(|v|) \frac{\langle u, v \rangle}{|u||v|} p(u, v) dudv > 0$$

260 for any $0 \neq h \in L^2(\rho)$.

Proof. The factor $\frac{2}{3}$ and the normalizing constant Z does not play a role in the above inequality, so we neglect them in the following proof. We only consider the case $\beta < 1$, since when $\beta = 1$ the Gaussian distribution neatly ensures strict positiveness of the integral operator through Taylor expansion of $\langle u, v \rangle e^{c\langle u, v \rangle}$. Note that

$$\begin{aligned} I &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(|u|)e^{-2|u|^{2\beta}} h(|v|)e^{-2|v|^{2\beta}} \frac{\langle u, v \rangle}{|u||v|} e^{|u|^{2\beta} + |v|^{2\beta} - |u - v|^{2\beta}} dudv \\ &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|)\tilde{h}(|v|) \frac{\langle u, v \rangle}{|u||v|} e^{\Phi_2(u, v)} dudv, \end{aligned}$$

where $\tilde{h}(r) := h(r)e^{-2r^{2\beta}}$ and

$$\Phi_2(u, v) := |u|^{2\beta} + |v|^{2\beta} - |u - v|^{2\beta}.$$

By Lemma 4.4, $|u - v|^{2\beta}$ is negative definite. Then, by Theorem 5.4, $\Phi_2(u, v)$ is positive definite. Thus, by Lemma 4.5 with $\Phi_1(u, v) = \langle u, v \rangle$ and $\Phi_2(u, v)$ as above, we have

$$\begin{aligned} I &\geq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) \frac{\langle u, v \rangle}{|u||v|} (|u|^{2\beta} + |v|^{2\beta} - |u - v|^{2\beta}) dudv \\ &= - \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) \frac{\langle u, v \rangle}{|u||v|} |u - v|^{2\beta} dudv =: \tilde{I}, \end{aligned} \quad (4.5)$$

where in the equality we dropped the term $|u|^\beta + |v|^\beta$ because, due to symmetry of $\langle u, v \rangle$,

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} g_1(|u|) g_2(|v|) \frac{\langle u, v \rangle}{|u||v|} = 0$$

for any $g_1, g_2 \in L^2(\rho)$. We shall use this property several times in the following.

Next, we use Gamma function to bound \tilde{I} in (4.5) from below by a Gaussian kernel as in the previous section. Note that for any $x > 0$ and $\beta < 1$,

$$|u - v|^{2\beta} = \frac{\beta}{\Gamma(1 - \beta)} \int_0^\infty (1 - e^{-\lambda|u - v|^2}) \frac{d\lambda}{\lambda^{\beta+1}}.$$

Plugging this into the integral in (4.5), and using the symmetry of $\langle u, v \rangle$ again, we obtain

$$\begin{aligned} \tilde{I} &= \frac{\beta}{\Gamma(1 - \beta)} \int_0^\infty \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) \frac{\langle u, v \rangle}{|u||v|} (e^{-\lambda|u - v|^2} - 1) dudv \frac{d\lambda}{\lambda^{\beta+1}} \\ &= \frac{\beta}{\Gamma(1 - \beta)} \int_0^\infty \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) \frac{\langle u, v \rangle}{|u||v|} e^{-\lambda|u - v|^2} dudv \frac{d\lambda}{\lambda^{\beta+1}} \\ &= \frac{\beta}{\Gamma(1 - \beta)} \int_0^\infty \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) e^{-\lambda(|u|^2 + |v|^2)} \frac{\langle u, v \rangle}{|u||v|} e^{2\lambda\langle u, v \rangle} dudv \frac{d\lambda}{\lambda^{\beta+1}}. \end{aligned}$$

By the symmetry of $\langle u, v \rangle$ and Taylor expansion of $e^{2\lambda\langle u, v \rangle}$, we have

$$\begin{aligned} \tilde{I} &= \frac{\beta}{\Gamma(1 - \beta)} \int_0^\infty \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) e^{-\lambda(|u|^2 + |v|^2)} \frac{\langle u, v \rangle}{|u||v|} \sum_{n=0}^\infty \frac{\langle u, v \rangle^{2n+1}}{(2n+1)!} dudv 2^{2n+1} \lambda^{2n-\beta} d\lambda \\ &= \sum_{n=0}^\infty \frac{\beta}{\Gamma(1 - \beta)} \int_0^\infty \int_0^\infty \int_0^\infty \tilde{h}(r) \tilde{h}(s) e^{-\lambda(r^2 + s^2)} (rs)^{d+2n+1} C_n dr ds \lambda^{2n-\beta} d\lambda, \end{aligned}$$

265 where we denote $C_n := \int_{\xi \in S^{d-1}} \int_{\eta \in S^{d-1}} \frac{2^{2n+1} \langle \xi, \eta \rangle^{2n+2}}{(2n+1)!} d\xi d\eta$, which is positive. Thus,

$$\begin{aligned} \tilde{I} &= \sum_{n=0}^\infty \frac{C_n \beta}{\Gamma(1 - \beta)} \int_0^\infty \lambda^{2n-\beta} \left[\int_0^\infty \tilde{h}(r) e^{-\lambda r^2} r^{d+2n+1} dr \right]^2 d\lambda \\ &\geq \sum_{n=0}^\infty \frac{C_n \beta}{\Gamma(1 - \beta)} \int_1^\infty \lambda^{2n-\beta} d\lambda \left[\int_0^\infty \tilde{h}(r) e^{-\lambda r^2} r^{d+2n+1} dr \right]^2. \end{aligned}$$

Note that $\tilde{C}_{n,\beta} = \frac{C_n \beta}{\Gamma(1 - \beta)} \int_1^\infty \lambda^{2n-\beta} d\lambda > 0$ for each $n \geq 0$. Combing all the above, we have

$$I \geq \sum_{n=0}^\infty \tilde{C}_{n,\beta} \left[\int_0^\infty h(r) e^{-2r^{2\beta} - 2r^2} r^{d+2n+1} dr \right]^2,$$

which is positive if $h \neq 0 \in L^2(f)$ with $f(r) := r^{d+1} e^{-2r^{2\beta} - 2r^2}$, because by Lemma 5.9, the set of functions $\text{span}\{1, r^2, r^4, \dots\}$ is complete in $L^2(\mathbb{R}^+, f)$. Note that $\text{supp } f = \text{supp } \rho = \mathbb{R}^+$, so $h \neq 0 \in L^2(f)$ when $h \neq 0 \in L^2(\rho)$. We conclude the proof. ■

The coercivity condition follows directly from the above proposition.

Theorem 4.7. *Let $\Phi(r) = r^{2\beta}$ for $\beta \in [1/2, 1]$. Then the coercivity condition holds true for the system (2.1) with $N = 3$ and with an initial distribution such that the joint distribution of $(\mathbf{r}_{12}^0, \mathbf{r}_{13}^0)$ is $p(u, v)$ in (4.1).*

Proof. Since $\beta \in [1/2, 1]$ and the initial distribution of $(\mathbf{r}_{12}^0, \mathbf{r}_{13}^0)$ is $p(u, v)$, it follows from Proposition 4.1 that the process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$ is stationary with distribution $p(u, v)$. Then, the coercivity condition is equivalent to that

$$I := \mathbb{E}[h(|\mathbf{r}_{12}^t|)h(|\mathbf{r}_{13}^t|)\frac{\langle \mathbf{r}_{12}^t, \mathbf{r}_{13}^t \rangle}{|\mathbf{r}_{12}^t||\mathbf{r}_{13}^t|}] > 0$$

for any $h \neq 0 \in L^2(\rho)$, where ρ is the stationary probability density of $|\mathbf{r}_{12}^t|$. Note that

$$I = \frac{1}{Z} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(|u|)h(|v|)\frac{\langle u, v \rangle}{|u||v|} e^{-\frac{2}{3}(|u|^{2\beta} + |v|^{2\beta} + |u-v|^{2\beta})} dudv.$$

Then we can conclude the theorem by Proposition 4.6. ■

Remark 4.8. *We point out that requirement $\beta \in (0, 1]$ is to ensure that the stationary density $p(u, v)$ is a positive definite kernel. When $\beta > 1$, the above method does no longer work, because $p(u, v)$ is not positive definite as shown in Lemma 4.4. The requirement $\beta \geq \frac{1}{2}$ is to ensure that the drift term is continuous, so that a strong solution exists. When $\beta < \frac{1}{2}$, drift is moderately singular, the existence of a solution is open [23, 17], but the coercivity inequality still holds true.*

4.3. General interaction potentials

The “comparison to a Gaussian kernel” technique in Lemma 4.5 and Proposition 4.6 can be generalized to prove the coercivity condition for a large class of interaction functions. The following lemma provides the key element in such a generalization.

Assumption 4.9. *Assume that $\Phi : \mathbb{R}^+ \rightarrow \mathbb{R}$ can be decomposed as*

$$\Phi(r) = \Phi_0(r) + ar^{2\beta},$$

where $\Phi_0 \in C^1(\mathbb{R}^+, \mathbb{R}^+)$ is a function such that $\Phi_0(|u-v|)$ is a negative definite kernel, $a > 0$ and $\beta \in [1/2, 1]$. Assume further that

$$Z := \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{-\frac{1}{3}[\Phi(|u|) + \Phi(|v|) + \Phi(|u-v|)]} dudv < \infty.$$

Lemma 4.10. *Let $\Phi : \mathbb{R}^+ \rightarrow \mathbb{R}$ be a function satisfying Assumption 4.9 and let $\rho(r)$ be the density of $|U|$ with (U, V) having a joint distribution $p(u, v) = \frac{1}{Z} e^{-\frac{2}{3}[\Phi(|u|) + \Phi(|v|) + \Phi(|u-v|)]}$. Then,*

$$I = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} h(|u|)h(|v|)\frac{\langle u, v \rangle}{|u||v|} e^{-[\Phi(|u|) + \Phi(|v|) + \Phi(|u-v|)]} dudv > 0$$

for any $0 \neq h \in L^2(\rho)$.

Proof. Rewrite the integral as

$$\begin{aligned} I &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} [h(|u|)e^{-\frac{2}{3}\Phi(|u|)}][h(|v|)e^{-\frac{2}{3}\Phi(|v|)}]\frac{\langle u, v \rangle}{|u||v|} e^{-\frac{2}{3}a|u-v|^{2\beta} - \frac{2}{3}\Phi_0(|u-v|)} dudv \\ &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|)\tilde{h}(|v|)\frac{\langle u, v \rangle}{|u||v|} e^{-\frac{2}{3}a|u-v|^{2\beta} + \frac{2}{3}\tilde{\Phi}(|u-v|)} dudv, \end{aligned}$$

where $\tilde{h}(r) = h(r)e^{-\frac{2}{3}\Phi(r) - \frac{2}{3}\Phi_0(r)}$ and

$$\tilde{\Phi}(u, v) := \Phi_0(|u|) + \Phi_0(|v|) - \Phi_0(|u-v|).$$

Since $\Phi_0(|u-v|)$ is negative definite, by Theorem 5.3, $\tilde{\Phi}(u, v)$ is positive definite. Also, by Lemma 4.4, $\langle u, v \rangle e^{-\frac{2}{3}a|u-v|^{2\beta}}$ is positive definite. Hence, by Lemma 4.5, we have

$$I \geq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{h}(|u|) \tilde{h}(|v|) \frac{\langle u, v \rangle}{|u||v|} e^{-\frac{2}{3}a|u-v|^{2\beta}} du dv.$$

Then the strict positive definiteness follows from Proposition 4.6. ■

Remark 4.11. The above lemma can be directly generalized to non-radial kernels of the form

$$\Phi(u, v) = \Phi_0(u, v) + c|u-v|^{2\beta}$$

with $\Phi_0(u, v)$ being negative definite, $c > 0$, and with $\beta \in (0, 1]$.

The coercivity condition follows directly from the above proposition.

Theorem 4.12. The coercivity condition holds true for the system (2.1) with $N = 3$ starting from an initial distribution such that the joint distribution of $(\mathbf{r}_{12}^0, \mathbf{r}_{13}^0)$ is $p(u, v)$ in (4.1), and with $\Phi : \mathbb{R}^+ \rightarrow \mathbb{R}$ satisfying Assumption 4.9.

Proof. Since $\beta \in [1/2, 1]$ and Φ_0 is smooth, the and the initial condition has distribution $p(u, v)$, the solution of the system leads to a stationary process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$. Then, the coercivity condition holds by Lemma 4.10. ■

We provide a few examples of negative definite radial kernels, and related positive kernels.

Lemma 4.13. For $0 < \alpha \leq 2$, $0 < \gamma \leq 1$ and $a \geq 0$, the following kernels are negative definite:

$$\begin{aligned} \Phi_1(|u-v|) &= (a + |u-v|^\alpha)^\gamma; \\ \Phi_2(|u-v|) &= \log[1 + (a + |u-v|^\alpha)^\gamma]. \end{aligned}$$

For any $c > 0$ and any integer $k \geq 1$, the following kernels are positive definite:

$$e^{-c\Phi_1(|u-v|)}, e^{-c\Phi_2(|u-v|)}, \Phi_2(|u-v|)^{-k}$$

Proof. By Lemma 4.4, if $0 \leq \alpha \leq 2$, then $|u-v|^\alpha$ is a negative definite kernel. By definition of a negative definite kernel $a + |u-v|^\alpha$ is also negative definite for any $a \in \mathbb{R}$. By Theorem 5.6, $\Phi_1(|u-v|) = (a + |u-v|^\alpha)^\gamma$ is also a negative definite kernel when $0 < \gamma \leq 1$ and $a \geq 0$.

Since $\Phi_1(|u-u|) = a^\gamma \geq 0$, by Theorem 5.6, $\log(1 + \Phi_1(|u-v|)) = \Phi_2(|u-v|)$ is negative definite.

The positive definiteness of $e^{-c\Phi_1(|u-v|)}$ and $e^{-c\Phi_2(|u-v|)}$ follows directly from Theorem 5.5. The kernel $\Phi_2(|u-v|)^{-k}$ is positive definite because

$$\int_0^\infty e^{-s\Phi_2(|u-v|)} ds = \frac{1}{\Phi_2(|u-v|)}$$

and because that the product of positive definite kernels are positive definite. ■

Proposition 4.14. Assume that the series

$$\Phi_1(r) = c_0 + \sum_{j=1}^{\infty} c_j \log[1 + (a_j + r^{\alpha_j})^{\gamma_j}] - \sum_{j=-1}^{-\infty} c_j [\log(1 + (a_j + r^{\alpha_j})^{\gamma_j})]^{-k_j} \quad (4.6)$$

$$\Phi_2(r) = \sum_{i=1}^{\infty} c'_i [(a'_i + r^{\alpha'_i})^{\gamma'_i}] - \sum_{i=-1}^{-\infty} c'_i [1 + (a'_i + r^{\alpha'_i})^{\gamma'_i}]^{-\beta_i} \quad (4.7)$$

converge for every $r \in \mathbb{R}^+$, where the coefficients satisfy the following conditions

1. $a_j \geq 0, a'_i \geq 0, c_j \geq 0, c'_i \geq 0$ for $i, j \neq 0$ and
2. $0 < \gamma_i \leq 1, \alpha_j, \alpha'_i \in [1, 2]$ for $i, j \neq 0$, and

3. $\beta_j > 0$ and $k_j \geq 1$ is a positive integer for each j .

Let $K : \mathbb{R}^+ \times \mathbb{R}^+ \rightarrow \mathbb{R}$ be an integral kernel defined in (4.4) with $p(u, v)$ defined in (4.1) and with

$$\Phi(r) = \Phi_1(r) + \Phi_2(r). \quad (4.8)$$

Then $K(r, s)$ is a positive definite kernel. Furthermore, if there exists $i_0 \geq 1$, such that

$$a'_{i_0} = 0, \quad \gamma'_{i_0} = 1, \quad \text{and} \quad c'_{i_0} > 0, \quad (4.9)$$

then the coercivity condition holds true for the system (2.1) with potential Φ in (4.8), if it starts from an initial distribution such that the joint distribution of $(\mathbf{r}_{12}^0, \mathbf{r}_{13}^0)$ is $p(u, v)$ in (4.1).

Proof. It follows directly from Lemma 4.13 that K is positive definite. Note that with the above conditions, the drift term is smooth and dominated by a term $r^{2\beta}$ with $\beta = \alpha'_{i_0}/2 \in [1/2, 1]$, so the system leads to a stationary process $(\mathbf{r}_{12}^t, \mathbf{r}_{13}^t)$. It follows from Lemma 4.10 that the coercivity condition holds true. ■

5. Appendix

5.1. Positive definite integral kernels

In this section, we review the definitions of positive and negative definite kernels, as well as their basic properties. The following definition is a real version of the definition in [26, p.67].

Definition 5.1. Let X be a nonempty set. A function $\phi : X \times X \rightarrow \mathbb{R}$ is called a (real) positive definite kernel if and only if it is symmetric (i.e. $\phi(x, y) = \phi(y, x)$) and

$$\sum_{j,k=1}^n c_j c_k \phi(x_j, x_k) \geq 0 \quad (5.1)$$

for all $n \in \mathbb{N}$, $\{x_1, \dots, x_n\} \in X$ and $\{c_1, \dots, c_n\} \in \mathbb{R}$. We call the function ϕ a (real) negative definite kernel if and only if it is symmetric and

$$\sum_{j,k=1}^n c_j c_k \phi(x_j, x_k) \leq 0 \quad (5.2)$$

for all $n \geq 2$, $\{x_1, \dots, x_n\} \in X$ and $\{c_1, \dots, c_n\} \in \mathbb{R}$ with $\sum_{j=1}^n c_j = 0$.

Remark. In the definition of positive definiteness in [26, p.67], a function $\phi : X \times X \rightarrow \mathbb{C}$ is positive definite if and only if

$$\sum_{j,k=1}^n c_j \bar{c}_k \phi(x_j, x_k) \geq 0 \quad (5.3)$$

for all $n \in \mathbb{N}$, $\{x_1, \dots, x_n\} \in X$ and $\{c_1, \dots, c_n\} \in \mathbb{C}$, where \bar{c} denotes the complex conjugate of a complex number c . It is straightforward to check that when ϕ is real-valued and symmetric, the definitions (5.1) and (5.3) are equivalent. Similarly, In the definition of negative definiteness in [26, p.67], a function $\phi : X \times X \rightarrow \mathbb{C}$ is negative definite if and only if it is Hermitian (i.e. $\phi(x, y) = \overline{\phi(y, x)}$) and

$$\sum_{j,k=1}^n c_j \bar{c}_k \phi(x_j, x_k) \leq 0 \quad (5.4)$$

for all $n \geq 2$, $\{x_1, \dots, x_n\} \in X$ and $\{c_1, \dots, c_n\} \in \mathbb{C}$ with $\sum_{j=1}^n c_j = 0$. We can again check that when ϕ is real-valued, the definitions (5.2) and (5.4) are equivalent. In this paper, we only consider real-valued, symmetric kernels.

Theorem 5.2 (Properties of positive definite kernels). Suppose that $k, k_1, k_2 : \mathcal{X} \times \mathcal{X} \subset \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ are positive definite kernels. Then

1. $c_1 k_1 + c_2 k_2$ is positive definite, for $c_1, c_2 \geq 0$
2. $k_1 k_2$ is positive definite. ([26, p.69])
3. $\exp(k)$ is positive definite. ([26, p.70])
4. $k(f(u), f(v))$ is positive definite for any map $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$
5. Inner product $\langle u, v \rangle = \sum_{j=1}^d u_j v_j$ is positive definite ([26, p.73])
6. $f(u)f(v)$ is positive definite for any function $f : \mathcal{X} \rightarrow \mathbb{R}$ ([26, p.69]).
7. If $k(u, v)$ is measurable and integrable, then $\iint k(u, v) du dv \geq 0$ ([27, p.524])

Theorem 5.3. [26, Theorem 3.1.17] Let $\phi : X \times X \rightarrow \mathbb{R}$ be symmetric. Then ϕ is positive definite if and only if

$$\det(\phi(x_j, x_k)_{j,k \leq n}) \geq 0$$

for all $n \in \mathbb{N}$ and all $\{x_1, \dots, x_n\} \subseteq X$.

Theorem 5.4. [26, Lemma 3.2.1] Let X be a nonempty set, $x_0 \in X$ and let $\psi : X \times X \rightarrow \mathbb{R}$ be a symmetric kernel. Put $\phi(x, y) := \psi(x, x_0) + \psi(y, x_0) - \psi(x, y) - \psi(x_0, x_0)$. Then ϕ is positive definite if and only if ψ is negative definite.

Theorem 5.5. Let X be a nonempty set and let $\psi : X \times X \rightarrow \mathbb{R}$ be a kernel. Then ψ is negative definite if and only if $\exp(-t\psi)$ is positive definite for all $t > 0$.

Proof. The complex version of this theorem is proved in Theorem 3.2.2 of [26]. The real version can be proved in a similar way. ■

Theorem 5.6. If $\psi : X \times X \rightarrow \mathbb{R}$ is negative definite and $\psi(x, x) \geq 0$, then so are ψ^α for $0 < \alpha < 1$ and $\log(1 + \psi)$.

Proof. The complex version of this theorem is proved in Theorem 3.2.10 of [26]. The real version can be proved in a similar way. ■

Theorem 5.7. [26, Proposition 3.3.2] Let X be nonempty and $\psi : X \times X \rightarrow \mathbb{C}$ be negative definite. Assume $\{(x, y) \in X \times X, \psi(x, y) = 0\} = \{(x, x) : x \in X\}$, then $\sqrt{\psi}$ is a metric on X .

5.2. Müntz-type theorems on half-line

We recall first the following theorem on the completeness of $\{t^{a_n}\}$ in weighted L^2 space on unbounded domain (see [28, 29] and see [30, 31] for recent developments).

Theorem 5.8. Let a_k be positive numbers, such that $a_{k+1} - a_k \geq d > 0$, ($k = 1, 2, \dots$), and let

$$\log \psi(r) = \begin{cases} 2 \sum_{a_k < r} \frac{1}{a_k}, & \text{if } r > a_1 \\ \frac{2}{a_1}, & \text{if } r \leq a_1. \end{cases}$$

Then $\{e^{-t} t^{a_k}\}$ is complete in $L^2(0, \infty)$ if and only if

$$\int_1^\infty \frac{\psi(r)}{r} dr = \infty$$

Lemma 5.9. The set of functions $\{r^{2k}, k = 1, 2, \dots\}$ is complete in $L^2([0, \infty), \rho)$ for any probability density ρ such that $\sup_{r>0} \rho(r) e^{2r} < \infty$.

Proof. Let $a_k = 2k$ for $k = 1, 2, \dots$. We define the function $\log(\psi(r)) = 2 \sum_{a_k < r} \frac{1}{a_k}$, if $r > a_1$, and $\log(\psi(r)) = \frac{2}{a_1}$ if $r \leq a_1$. Note that $2 \sum_{a_k < r} \frac{1}{a_k} = \sum_{k=1}^{\lfloor r/2 \rfloor} \frac{1}{k} > \ln(\lfloor r/2 \rfloor)$. Then $\psi(r) \geq r$ and

$$\int_1^\infty \frac{\psi(r)}{r^2} = \infty.$$

We conclude that $\{e^{-t}t^{2k}, k = 1, 2, \dots\}$ is complete in $L^2(0, \infty)$ by Theorem 5.8.

To show that $\{r^{2k}, k = 1, 2, \dots\}$ is complete in $L^2(\rho)$, assume that $\langle h(r), r^{2k} \rangle_{L^2(\rho)} = 0$ for all $k \geq 1$. Then

$$\int_0^\infty h(r)\rho(r)e^r r^{2k} e^{-r} dr = \int_0^\infty h(r)r^{2k}\rho(r)dr = 0$$

for all k . This implies that $h(r)\rho(r)e^r = 0$ in $L^2[0, \infty)$ (note that $h(r)\rho(r)e^r \in L^2[0, \infty)$ because $\sup_{r>0} \rho(r)e^{2r} < \infty$). Hence $h(r)\rho(r) = 0$ almost everywhere, and $h = 0$ in $L^2([0, \infty), \rho)$. ■

5.3. Stationary measure for a gradient system

Lemma 5.10. Suppose $H : \mathbb{R}^n \rightarrow \mathbb{R}$ is locally Lipschitz and that $Z = \int_{\mathbb{R}^n} e^{-2H(x)} dx < \infty$. Then $p(x) = \frac{1}{Z} e^{-2H(x)}$ is an invariant density to gradient system

$$dX_t = -\nabla H(X_t)dt + dB_t,$$

where (B_t) is an n -dimensional standard Brownian motion.

Proof. It follows directly by showing that $p(x)$ is a stationary solution to the backward Kolmogorov equation, i.e.

$$\frac{1}{2} \Delta p + \nabla \cdot (p \nabla H) = 0.$$

■

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