

# On Feynman-Kac and particle Markov chain Monte Carlo models

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## Abstract

This article is concerned with the analysis of a new class of advanced particle Markov chain Monte Carlo algorithms recently introduced by C. Andrieu, A. Doucet, and R. Holenstein. We present a natural interpretation of these models in terms of well known unbiasedness properties of Feynman-Kac particle measures, and a new duality with many-body Feynman-Kac models. This new perspective sheds a new light on the foundations and the mathematical analysis of this class of models, including their propagation of chaos properties. In the process, we also present a new stochastic differential calculus based on geometric combinatorial techniques to derive explicit Taylor type expansions of the semigroup of a class of particle Markov chain Monte Carlo models around their invariant measures w.r.t. the population size of the auxiliary particle sampler. These results provide sharp quantitative estimates of the convergence properties of conditional particle Markov chain models, including sharp estimates of the contraction coefficient of conditional particle samplers, and explicit and non asymptotic  $\mathbb{L}_p$ -mean error decompositions of the law of the random states around the limiting invariant measure. The abstract framework develop in this article also allows to design new natural extensions of models including island type particle methodologies.

## 1 Introduction

In the last two decades, particle simulation techniques have become one of the most active contact points between Bayesian statistical inference and applied probability. Their range of applications goes from statistical machine learning, information theory, theoretical chemistry and quantum physics, financial mathematics, signal processing, risk analysis, and several other domains in engineering and computer sciences. In contrast to conventional Markov chain Monte Carlo methodologies, these particle methods are not based on sampling long runs of a judiciously chosen Markov chain with a prescribed target probability measure. A brief survey on these stochastic particle models is provided in section 2.

In a seminal article [2] C. Andrieu, A. Doucet, and R. Holenstein introduced a new way to combine Markov chain Monte Carlo methods (*abbreviated MCMC*) with Sequential Monte Carlo methodologies (*abbreviated SMC*). Some variants of this particle Gibbs type models where ancestors are resampled in a forward pass have been recently developed in F. Lindsten, T. Schön, M. I. Jordan in [38], and in the article [39] by F. Lindsten, T. Schön.

This new class of Monte Carlo samplers are termed particle Markov chain Monte Carlo methods (*abbreviated PMCMC*). These emerging particle sampling technologies are particularly important in signal processing and in Bayesian statistics. In this application area, they are used to estimate posterior distributions of unknown parameters when the likelihood functions are unknown or computationally untractable. Here, the central idea is to

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run a MCMC sampler and compute these likelihood functions using an auxiliary particle sampler. In this situation, the updates of the resulting particle MCMC samplers are defined on extended state spaces. Using the unbiased property of the particle likelihood function, the marginal of their invariant measure coincide with the desired posterior distribution.

In the last few years, these powerful PMCMC methodologies attracted considerable attention in a variety of application domains, including in statistical machine learning [5, 33, 38, 48], finance and econometrics [13, 25, 30, 40, 43], biology [31, 36, 44], computer sciences [32], environmental statistics [26, 27, 42], social networks analysis [29], signal processing [39, 41], forecasting and data assimilation [37, 35, 47], among other fields.

The convergence analysis of the PMCMC models has also been started in a series of articles [4, 9, 34, 38, 39]. The  $\phi$ -irreducibility and aperiodicity of PMCMC models was already discussed in the pionnering article by C. Andrieu, A. Doucet, R. Holenstein [2]. The first rather crude quantitative estimates of the convergence properties of PMCMC models has been presented by N. Chopin, S.S. Singh in [9], using a sophisticated coupling technology of ancestral particle paths. More refined contraction estimates have been recently obtained by C. Andrieu, A. Lee, M. Vihola [4] using an original and powerful doubly conditional type analysis of the normalizing particle constants. We also quote the independent article by F. Lindsten, R. Douc, E. Moulines [34] which provide similar quantitative estimates using lower bound estimates of PMCMC transition based on the stability of Feynman-Kac semigroups.

In all of these studies, the validity of PMCMC samplers is assessed by interpreting these models as a traditional MCMC sampler on a sophisticated and extended state space in which all the random variables generated by some particle model are seen as auxiliary variables. The target measure of these MCMC models are expressed in terms of a density involving compositions of random mappings encoding the full ancestral lineages of all the genetic type particle, from the origin up to the final time horizon.

These sophisticated target measures on extended spaces are often termed "artificial joint distributions" to underline the fact that they only have a instrumental technical role. Furthermore, in most of the studies dedicated to the convergence of PMCMC model the analysis is based on the derivation of judicious lower bound estimates of transitions probability. These estimates are used to conclude the uniform ergodicity of PMCMC type chains satisfying the well known minorization condition.

This article is concerned with an alternative probabilistic foundation of PMCMC methodologies. In the first part we provide an interpretation of PMCMC models in terms of a new duality relation between Feynman-Kac measures on path spaces and their many-body version. This duality relation can be seen as an extension of the well known unbiasedness properties of unnormalized particle measures to many-body Feynman-Kac models.

This natural viewpoint simplifies considerably the design and the convergence analysis of this class of particle models. From the numerical viewpoint, in the context of particle Gibbs type MCMC model (a.k.a conditional SMC updates) it also avoids to store at each time step the complete ancestral encoding of the frozen trajectory in the auxiliary particle sampler. Last but not least, this new formulation also allows to design new and natural classes of PMCMC based on island type models and particle Gibbs methodologies.

The second part of the article is concerned with the propagations of chaos properties of PMCMC models based on the sampling of a particle model with a frozen trajectory. We design explicit Taylor type expansions of the law of finite block of particles in terms of the population size of the auxiliary particle model. These expansions are naturally parametrized by decorated ("infected") forests. Their accuracy at any order is related naturally to the number of coalescent edges and the number of infections. To the best of our knowledge, these propagation of chaos expansions are the first result of this type for this class of particle Markov chain Monte Carlo.

As direct consequences, these expansions provide Taylor decompositions of the semigroup of conditional PMCMC models *around their invariant target measures* w.r.t. the precision

parameter  $1/N$ .

We also illustrate the impact of these expansions with sharp and non asymptotic expansions of the Dobrushin contraction coefficient of any iterated conditional PMCMC transitions. We also provide an explicit decomposition of the  $\mathbb{L}_p$ -distance between the law of the random states of a class of PMCMC model around the limiting invariant measure. These results can also be used to estimate the bias and the variance of the random states of a (non stationary) PMCMC model. Incidentally, the duality between Feynman-Kac models and their many-body versions allows to transfer these Taylor expansions to the original Feynman-Kac particle models.

Last but not least, the duality relation and differential calculus developed in this article also open an avenue of open research problems in the field of Feynman-Kac particle models and PMCMC methodologies.

The article is organized as follows:

In a preliminary section, section 2, we review some rather well know results on Feynman-Kac models and their mean field particle interpretations, including path space models and backward particle Markov chain measures. Paragraph 2.4 introduces many body Feynman-Kac models aiming at describing the collective motion of particles in usual Feynman-Kac models. These models will appear to be particularly well suited to the analysis of PMCMC samplers.

Section 3 is dedicated to conditional particle MCMC methodologies:

Paragraph 3.1 provide a transport equation and a new duality relation between many-body Feynman-Kac models and a conditional Feynman-Kac particle model with a frozen trajectory. Paragraph 3.2 is dedicated to historical particle models and their dual frozen particle models. For instance, we show that the conditional distribution of *the ancestral lines* of Feynman-Kac particle model w.r.t. its complete ancestral tree coincides with the backward particle distribution model.

In paragraph 3.3, we present two classes of PMCMC models: genealogical tree based samplers and backward sampling models. We also present three elementary proofs of the invariance properties of Feynman-Kac path measures w.r.t. these two classes of PMCMC models.

In section 3.4 we present a basic description of the Taylor expansions of conditional PMCMC transitions around their invariant measures. We also derive a series of important consequences of these expansions, including quantitative estimates of the stability properties of these models, and sharp estimates of the bias and the variance of the random states of the PMCMC Markov chain.

Section 4 is dedicated to the propagations of chaos properties of a conditional PMCMC particle model:

In the first paragraph, section 4.1, we have collected some combinatorial preliminaries on tensor products of empirical measures and their decorated version. Section 4.2 is concerned with Taylor expansions of  $q$ -tensor product of unnormalized particle measures.

The propagation of chaos properties and related Taylor expansions of frozen particle models are discussed in section 4.3.

Paragraph 4.4 is dedicated to the detailed description of these Taylor decompositions in terms of infected and coalescent forest expansions.

In the last section, section 5, we discuss some extensions and open questions. Paragraph 5.1 is concerned with the modeling and the analysis of a new class of island PMCMC samplers. Paragraph 5.2 is dedicated at stating some important open questions related to conditional particle MCMC models.

## 2 Feynman-Kac models: old and new

This introductory section collects first some basic notations used in this article. We recall then the definition and main properties of Feynman-Kac measures on their usual state and path spaces. The last paragraph introduces a particular Feynman-Kac model [46] well-suited to the mathematical analysis of PMCMC samplers. Although we will not develop further this point of view, the statistically-minded reader will note the analogy of the model with the ones familiar in  $U$ -statistics, in that it relies strongly on properties of symmetric functions on the space of samples of a target distribution.

### 2.1 Notations

Given some measurable space  $S$  we denote respectively by  $\mathcal{M}(S)$ ,  $\mathcal{P}(S)$  and  $\mathcal{B}(S)$ , the set of signed measures on  $S$ , the convex subset of probability measures, and the Banach space of bounded measurable functions equipped with the uniform norm  $\|f\| = \sup_{x \in S} |f(x)|$ .

The total variation norm on measures  $\mu \in \mathcal{M}(S)$  is defined by

$$\|\mu\|_{tv} = \sup_{f \in \mathcal{B}(S) : \|f\| \leq 1} |\mu(f)| \quad \text{with the Lebesgue integral} \quad \mu(f) := \int \mu(dx) f(x)$$

We also denote by  $\delta_a$  the Dirac measure at some state  $a$ , so that  $\delta(f) = f(a)$ . We say that  $\nu \leq \mu$  as soon as  $\nu(f) \leq \mu(f)$  for any non negative function  $f$ .

A bounded integral operator  $Q(x, dy)$  between the measurable spaces  $S$  and  $S'$  is defined for any  $f \in \mathcal{B}(S')$  by the measurable function  $Q(f) \in \mathcal{B}(S)$  defined by

$$Q(f)(x) := \int Q(x, dy) f(y)$$

The operator  $Q$  generates a dual operator  $\mu \in \mathcal{M}(S) \mapsto \mu Q \in \mathcal{M}(S')$  by the dual formula  $(\mu Q)(f) = \mu(Q(f))$ .

When a bounded integral operator  $M$  from a state space  $S$  into a possibly different state space  $S'$  has a constant mass, that is, when  $M(1)(x) = M(1)(y)$  for any  $(x, y) \in S^2$ , the operator  $\mu \mapsto \mu M$  maps the set  $\mathcal{M}_0(S)$  of measures  $\mu$  on  $S$  with null mass  $\mu(1) = 0$  into  $\mathcal{M}_0(S')$ . In this situation, we let  $\beta(M)$  be the Dobrushin coefficient of a bounded integral operator  $M$  defined by the formula  $\beta(M) := \sup \{\text{osc}(M(f)) ; f : \text{osc}(f) \leq 1\}$ , where  $\text{osc}(f) := \sup_{x, y} |f(x) - f(y)|$  stands for the oscillation of some function.

When  $M$  is a Markov transition,  $\beta(M)$  coincides with the Dobrushin contraction parameter (a.k.a. the Dobrushin ergodic coefficient) defined by

$$\beta(M) = \sup_{\mu, \nu} (\|\mu M - \nu M\|_{tv} / \|\mu - \nu\|_{tv}) = \sup_{x, y} \|M(x, \cdot) - M(y, \cdot)\|_{tv}$$

The  $q$ -tensor product of  $Q$  is the integral operator defined for any  $f \in \mathcal{B}(S^q)$  by

$$Q^{\otimes q}(f)(x^1, \dots, x^q) := \int \left\{ \prod_{1 \leq i \leq q} Q(x^i, dy^i) \right\} f(y^1, \dots, y^q)$$

We also denote by  $Q_1 Q_2$  the composition of two operators defined by

$$(Q_1 Q_2)(x, dz) = \int Q_1(x, dy) Q_2(y, dz)$$

The Boltzmann-Gibbs transformation  $\Psi_G : \eta \in \mathcal{P}(S) \mapsto \Psi_G(\eta) \in \mathcal{P}(S)$  associated with some positive function  $G$  on some state space  $S$  is defined by

$$\Psi_G(\eta)(dx) = \frac{1}{\eta(G)} G(x) \eta(dx)$$

We also denote by  $\#(E)$  the cardinality of a finite set and we use the standard conventions  $(\sup_{\emptyset}, \inf_{\emptyset}) = (-\infty, +\infty)$ , and  $(\sum_{\emptyset}, \prod_{\emptyset}) = (0, 1)$ .

We will also consider the notion of differential for sequences of measures introduced in [22]. We let  $\mu^N$  be a uniformly bounded sequence of measures on  $\mathcal{M}(S)$  in the sense that  $\sup_{N \geq 1} \|\mu^N\| < \infty$ . The sequence  $\mu^N$  is said to converge strongly to some measure  $\mu \in \mathcal{M}(S)$ , as  $N \uparrow \infty$  if we have  $\lim_{N \uparrow \infty} \mu^N(f) = \mu(f)$ , for any  $f \in \mathcal{B}(S)$ . In this case, the discrete derivative of  $\mu^N$  is defined by

$$\partial \mu^N = N (\mu^N - \mu)$$

We say that  $\mu^N$  is differentiable whenever  $\partial \mu^N$  is uniformly bounded and it strongly converge to some signed measure  $d^{(1)}\mu$ , as  $N \uparrow \infty$ . When  $\partial \mu^N$  is differentiable, with a discrete derivative writtem  $\partial^{(2)}\mu^N$  we can define its derivative, denoted by  $d^{(2)}\mu$ , and so on. A mapping  $N \mapsto \mu^N$  that is differentiable up to some order  $l$  can be written in the following form

$$\mu^N = \sum_{0 \leq k \leq l} \frac{1}{N^k} d^{(k)}\mu + \frac{1}{N^{l+1}} \partial^{(l+1)}\mu^N$$

with the convention  $d^{(0)}\mu = \mu$ . We easily extend these definitions to sequence of integral operators  $Q^N$  and sequence of functions  $f^N$ . In this situation, we denote by  $d^{(l)}Q$  and  $d^{(l)}f$  the corresponding differentials.

## 2.2 Mean field particle models

Given some measurable space  $S$  we denote respectively by  $\mathcal{P}(S)$  and  $\mathcal{B}(S)$ , the set of probability measures on  $S$ , and the Banach space of bounded measurable functions equipped with the uniform norm.

We consider a collection of bounded and non negative potential functions  $G_n$  on some measurable state spaces  $S_n$ , with  $n \in \mathbb{N}$ . To avoid unnecessary technical discussions, we also assume that the functions  $G_n$  are chosen s.t.  $g_n := \inf_{x,y} (G_n(x)/G_n(y)) > 0$  for any  $n \geq 0$ . The extension of the results presented in this article to more general models, including indicator type functions and unbounded potential functions, can be analyzed using the methodologies developed in [15] (see for instance section 2.3, 2.4, 3.5.2, and section 7.2.2).

We also let  $X_n$  be a Markov chain on  $S_n$  with initial distribution  $\eta_0 \in \mathcal{P}(S_0)$  and some Markov transitions  $M_n$  from  $S_{n-1}$  into  $S_n$ . The Feynman-Kac measures  $(\eta_n, \gamma_n)$  associated with the parameters  $(G_n, M_n)$  are defined for any  $f_n \in \mathcal{B}(S_n)$  by

$$\eta_n(f_n) := \gamma_n(f_n)/\gamma_n(1) \quad \text{with} \quad \gamma_n(f_n) = \mathbb{E} \left( f_n(X_n) \prod_{0 \leq p < n} G_p(X_p) \right) \quad (2.1)$$

The evolution equations associated with these measures are given by

$$\gamma_{n+1} = \gamma_n Q_{n+1} \quad \text{and} \quad \eta_{n+1} = \Phi_{n+1}(\eta_n) := \Psi_{G_n}(\eta_n) M_{n+1} \quad (2.2)$$

with the integral operators

$$Q_{n+1}(x_n, dx_{n+1}) = G_n(x_n) M_{n+1}(x_n, dx_{n+1})$$

The unnormalized measures  $\gamma_n$  can be expressed in terms of the normalized ones using the well known product formula

$$\gamma_n(f_n) = \eta_n(f_n) \prod_{0 \leq p < n} \eta_p(G_p)$$

We also recall the semigroup decompositions

$$\forall 0 \leq p \leq n \quad \gamma_n = \gamma_p Q_{p,n} \quad \text{and} \quad \eta_n = \eta_p \overline{Q}_{p,n}$$

with the integral operators  $Q_{p,n} = Q_{p+1} \dots Q_n$ , and the normalized semigroups

$$\overline{Q}_{p,n}(f_n)(x_p) = Q_{p,n}(f_n)(x_p) / \eta_p Q_{p,n}(1) = \overline{Q}_{p+1} \dots \overline{Q}_n$$

In the above display,  $\overline{Q}_{p+1}$  stands for the collection of integral operators defined as  $Q_{p+1}$  by replacing  $G_p$  with the normalized potential functions  $\overline{G}_p = G_p / \eta_p(G_p)$ .

The mean field particle interpretation of the measures  $(\eta_n, \gamma_n)$  starts with  $N$  independent random variables  $\xi_0^{(N)} := (\xi_0^{(N,i)})_{1 \leq i \leq N} \in S_0^N$  with common law  $\eta_0$ . The simplest way to evolve the population of  $N$  individual (a.k.a. samples, particle, or walkers)  $\xi_n^{(N)} := (\xi_n^{(N,i)})_{1 \leq i \leq N} \in S_n^N$  is to consider  $N$  conditionally independent individuals  $\xi_{n+1}^{(N)} := (\xi_{n+1}^{(N,i)})_{1 \leq i \leq N} \in S_{n+1}^N$  with common distribution

$$\Phi_{n+1}(m(\xi_n^{(N)})) \quad \text{with} \quad m(\xi_n^{(N)}) := \frac{1}{N} \sum_{1 \leq i \leq N} \delta_{\xi_n^{(N,i)}} \quad (2.3)$$

This particle model (2.3) is a genetic type particle model with a selection and a mutation transition dictated by the potential function  $G_n$  and the Markov transition  $M_n$ .

Loosely speaking, the model functions recursively as follows: starting from a sample  $\xi_0^{(N)}$  at  $t = 0$  of the initial distribution  $\eta_0$  (so that  $m(\xi_0^{(N)}) \simeq_{N \uparrow \infty} \eta_0$ ), and assuming  $m(\xi_n^{(N)}) \simeq_{N \uparrow \infty} \eta_n$ , then the population at time  $(n+1)$  is formed with  $N$  "almost" independent samples w.r.t.  $\eta_{n+1}$  so that  $m(\xi_{n+1}^{(N)}) \simeq_{N \uparrow \infty} \eta_{n+1}$ . The reader is referred to [15] for details.

In the further development of the article, the size  $N$  and the precision of the particle model will be fixed. Thus, to clarify the presentation, when there are no possible confusions we suppress the index parameter  $N$  and we write  $\xi_n$  and  $\xi_n^i$  instead of  $\xi_n^{(N)}$  and  $\xi_n^{(N,i)}$ .

### 2.3 Path space models

To illustrate the generality of the Feynman-Kac models discussed above, let us replace the 5-tuple  $(G_n, M_n, Q_n, S_n, X_n)$  by its path-space analog  $(\mathbf{G}_n, \mathbf{M}_n, \mathbf{Q}_n, \mathbf{S}_n, \mathbf{X}_n)$ . That is, in the constructions of the previous paragraph, each item of the first 5-tuple is going to be replaced by its path space analog:  $\mathbf{X}_n$  is the historical process associated to  $X_n$ ,

$$\mathbf{X}_n := (X_0, \dots, X_n) \in \mathbf{S}_n := (S_0 \times \dots \times S_n). \quad (2.4)$$

We write  $\mathbf{M}_n$  for the Markov transition of  $\mathbf{X}_n$ . The functions  $\mathbf{G}_n$  on  $\mathbf{S}_n$  only depend on the last coordinate and are defined by  $\mathbf{G}_n(\mathbf{X}_n) := G_n(X_n)$ .

In general, in the article, a bold symbol will denote an element, function, measure... on a path space, even when the latter is considered as a state space –as in the present paragraph. In particular, we let  $(\boldsymbol{\gamma}_n, \boldsymbol{\eta}_n, \boldsymbol{\xi}_n)$  be the Feynman-Kac measures and the particle model defined as  $(\gamma_n, \eta_n, \xi_n)$ , by replacing  $(G_n, M_n, Q_n, S_n, X_n)$  by  $(\mathbf{G}_n, \mathbf{M}_n, \mathbf{Q}_n, \mathbf{S}_n, \mathbf{X}_n)$ . The two measures on the state space  $\mathbf{S}_n$  are given for any  $\mathbf{f}_n \in \mathcal{B}(\mathbf{S}_n)$  by

$$\boldsymbol{\eta}_n(\mathbf{f}_n) := \boldsymbol{\gamma}_n(\mathbf{f}_n) / \boldsymbol{\gamma}_n(\mathbf{1}) \quad \text{with} \quad \boldsymbol{\gamma}_n(\mathbf{f}_n) = \mathbb{E} \left( \mathbf{f}_n(\mathbf{X}_n) \prod_{0 \leq p < n} \mathbf{G}_p(\mathbf{X}_p) \right). \quad (2.5)$$

By construction,  $(\boldsymbol{\gamma}_n, \boldsymbol{\eta}_n)$  are the  $S_n$  marginals of the measures  $(\boldsymbol{\gamma}_n, \boldsymbol{\eta}_n)$ . The same property holds at the level of the particles of the two models. To be more precise, we observe that the  $i$ -th path space particle

$$\boldsymbol{\xi}_n^i = (\xi_{0,n}^i, \xi_{1,n}^i, \dots, \xi_{n,n}^i) \in \mathbf{S}_n := (S_0 \times \dots \times S_n)$$

of the particle model  $\xi_n$  can be interpreted as the line of ancestors  $\xi_{p,n}^i$  of the  $i$ -th individual  $\xi_{n,n}^i$  at time  $n$ , at every level  $0 \leq p \leq n$ , with  $1 \leq i \leq N$ . This shows that the particle model  $\xi_n = (\xi_n^i)_{1 \leq i \leq N}$  coincides with the evolution of the individuals  $\xi_{n,n} = (\xi_{n,n}^i)_{1 \leq i \leq N}$ . The path space model  $\xi_n$  is called the genealogical tree model associated with the particle system  $\xi_n$ .

To distinguish these two Feynman-Kac models we adopt the following terminology. The 3-tuple  $(\eta_n, \gamma_n, \xi_n)$  is called the Feynman-Kac particle model associated with the potential functions  $G_n$  and the Markov transitions  $M_n$  on the state spaces  $S_n$ . The path space model  $(\gamma_n, \eta_n, \xi_n)$  is called the historical version of  $(\gamma_n, \eta_n, \xi_n)$ .

Whenever the integral operators  $Q_n$  have some densities  $H_n$  w.r.t. some reference distributions  $\nu_n$  on  $S_n$ , the path space measure  $\eta_n$  can be expressed in terms of the marginal measures  $(\eta_p)_{0 \leq p \leq n}$  using the well known backward formula

$$\eta_n(d\mathbf{x}_n) = \eta_n(dx_n) \prod_{1 \leq k \leq n} \mathbb{L}_{k, \eta_{k-1}}(x_k, dx_{k-1}) \quad (2.6)$$

with the collection of Markov transitions  $\mathbb{L}_{n+1, \eta_n}$  from  $S_{n+1}$  into  $S_n$  defined by

$$\mathbb{L}_{n+1, \eta_n}(x_{n+1}, dx_n) = \eta_n(dx_n) H_{n+1}(x_n, x_{n+1}) / \eta_n(H_{n+1}(\cdot, x_{n+1})) \quad (2.7)$$

In the above displayed formula,  $d\mathbf{x}_n = d(x_0, \dots, x_n)$  stands for an infinitesimal neighborhood of a trajectory  $\mathbf{x}_n = (x_0, \dots, x_n) \in \mathcal{S}_n := (S_0 \times \dots \times S_n)$ .

In this setting, the two unbiased estimates of  $\gamma_n$  are defined by

$$\forall i = 1, 2 \quad \gamma_n^{(N, i)} = \left\{ \prod_{0 \leq p < n} m(\xi_p)(G_p) \right\} \eta_n^{(N, i)} \quad (2.8)$$

with the couple of random measures  $(\eta_n^{(N, 1)}, \eta_n^{(N, 2)})$  on  $\mathcal{S}_n$  defined by

$$\eta_n^{(N, 1)}(d\mathbf{x}_n) := m(\xi_n)(d\mathbf{x}_n) \quad \text{and} \quad \eta_n^{(N, 2)}(d\mathbf{x}_n) := m(\xi_n)(dx_n) \prod_{1 \leq k \leq n} \mathbb{L}_{k, m(\xi_{k-1})}(x_k, dx_{k-1}).$$

## 2.4 Many body Feynman-Kac models

### 2.4.1 Some terminology

We fix the size  $N$  of the particle model, and set  $\mathcal{S}_n := S_n^{[N]}$  for the  $N$ -th symmetric power of  $S_n$ :  $S_n^{[N]} := S_n \times \dots \times S_n / \Sigma_N = S_n^N / \Sigma_N$ , where we write  $\Sigma_N$  for the symmetric group of order  $N$ . The image in  $\mathcal{S}_n$  of an ordered sequence  $(x_1, \dots, x_n) \in S_n^N$  will be sometimes written with the set-theoretical notation  $\{x_1, \dots, x_n\}$  to emphasize that the order of the  $x_i$  does not matter, although we will also often identify  $(x_1, \dots, x_n)$  with its image in  $\mathcal{S}_n^{[N]}$  without further notice when no confusion can arise.

For example with this slight abuse of notation, noticing for further use that the particle model  $\xi_n$  can be viewed as a  $\mathcal{S}_n$ -valued Markov chain (since the distribution of the  $\xi_n^i$ ,  $i = 1 \dots N$  is  $\Sigma_N$ -invariant) we will have, for a function  $f$  on  $\mathcal{S}_n^{[N]}$ ,

$$f(\xi_n) := f(\{\xi_n^1, \dots, \xi_n^N\}) =: f(\xi_n^1, \dots, \xi_n^N).$$

In the further development of this section we use calligraphic letters such as  $x_n$  and  $y_n = \{y_n^i\}_{1 \leq i \leq N}$  to denote states in the product spaces  $\mathcal{S}_n = S_n^{[N]}$ , and slanted roman letters such as  $x_n, y_n, z_n$  to denote states in  $S_n$ . The path sequences in the product spaces  $\mathcal{S}_n := \prod_{0 \leq p \leq n} \mathcal{S}_p$  and  $\mathcal{S}_n := \prod_{0 \leq p \leq n} S_p$  are denoted by bold letters such as  $\mathbf{x}_n = (x_p)_{0 \leq p \leq n} \in \mathcal{S}_n$  and  $\mathbf{x}_n = (x_p)_{0 \leq p \leq n} \in \mathcal{S}_n$ . Finally, we also denote by  $dx_n = d\{x_n^1, \dots, x_n^N\}$ , resp.  $d\mathbf{x}_n = d(x_0, \dots, x_n)$ , the infinitesimal neighborhoods of a point  $x_n = \{x_n^i\}_{1 \leq i \leq N} \in \mathcal{S}_n = S_n^{[N]}$ , resp.  $\mathbf{x}_n = (x_p)_{0 \leq p \leq n} \in \mathcal{S}_n = \prod_{0 \leq p \leq n} \mathcal{S}_p$ .

### 2.4.2 Description of the models

We write  $\mathcal{M}_n$  for the Markov transitions of the particle model  $\chi_n := \xi_n$  viewed now as a *Markov chain* on  $\mathcal{S}_n$ , and introduce the potential functions  $\mathcal{G}_n(\chi_n) = m(\chi_n)(G_n)$ . We let  $(\Pi_n, \Gamma_n)$  be the Feynman-Kac measures on  $\mathcal{S}_n$  defined for any  $\mathcal{F}_n \in \mathcal{B}(\mathcal{S}_n)$  by

$$\Pi_n(\mathcal{F}_n) := \Gamma_n(\mathcal{F}_n)/\Gamma_n(1) \quad \text{with} \quad \Gamma_n(\mathcal{F}_n) = \mathbb{E} \left( \mathcal{F}_n(\chi_n) \prod_{0 \leq p < n} \mathcal{G}_p(\chi_p) \right) \quad (2.9)$$

Notice that the unbiasedness properties of  $\gamma_n^{(N,1)}(\mathbf{1})$  ensures that  $\Gamma_n(1) = \gamma_n(1)$ . Using (2.2) it is readily checked that

$$\Gamma_{n+1} = \Gamma_n \mathcal{Q}_{n+1} \quad \text{and} \quad \Pi_{n+1} := \Psi_{\mathcal{G}_n}(\Pi_n) \mathcal{M}_{n+1} \quad (2.10)$$

with the integral operators

$$\mathcal{Q}_{n+1}(x_n, dx_{n+1}) = \mathcal{G}_n(x_n) \mathcal{M}_{n+1}(x_n, dx_{n+1})$$

We denote by  $(\Pi_n, \Gamma_n)$  the Feynman-Kac measures associated with the historical process  $\mathbf{X}_n = (\chi_0, \dots, \chi_n)$ , and the potential functions  $\mathcal{G}_n(\mathbf{X}_n) := \mathcal{G}_n(\chi_n)$  on the path space  $\mathcal{S}_n$ . More formally, these measures are defined for any  $\mathcal{F}_n \in \mathcal{B}(\mathcal{S}_n)$  by

$$\Pi_n(\mathcal{F}_n) := \Gamma_n(\mathcal{F}_n)/\Gamma_n(\mathbf{1}) \quad \text{with} \quad \Gamma_n(\mathcal{F}_n) = \mathbb{E} \left( \mathcal{F}_n(\mathbf{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\chi_p) \right) \quad (2.11)$$

Whenever the integral operators  $\mathcal{Q}_n$  have some densities  $H_n$  w.r.t. some reference distributions  $\nu_n$  on  $S_n$ , given  $\mathbf{X}_n$  we let  $\mathbb{X}_n := (\mathbb{X}_p)_{0 \leq p \leq n}$  be a random path with conditional distribution

$$\mathcal{K}_n(\mathbf{X}_n, d\mathbf{x}_n) := m(\chi_n)(dx_n) \prod_{1 \leq k \leq n} \mathbb{L}_{k,m}(\chi_{k-1})(x_k, dx_{k-1}) \quad (2.12)$$

In the above displayed formula  $d\mathbf{x}_n$  stands for an infinitesimal neighborhood of the path  $\mathbf{x}_n = (x_p)_{0 \leq p \leq n} \in \mathcal{S}_n$ , and  $\mathbb{L}_{k,m}(\chi_{k-1})$  are the Markov transitions defined in (2.7).

The unbiasedness properties of the measures  $\gamma_n^{(N,i)}$  are equivalent to the fact that for any  $(f_n, g_n) \in (\mathcal{B}(\mathcal{S}_n) \times \mathcal{B}(S_n))$ , we have

$$\begin{aligned} \mathbb{E} \left( f_n(\mathbb{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\chi_p) \right) &= \mathbb{E} \left( f_n(\mathbf{X}_n) \prod_{0 \leq p < n} G_p(\chi_p) \right) \\ \mathbb{E} \left( f_n(\mathbb{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\chi_p) \right) &= \mathbb{E} \left( f_n(\mathbf{X}_n) \prod_{0 \leq p < n} G_p(\chi_p) \right) \end{aligned} \quad (2.13)$$

We emphasize that (2.13) holds true for general Feynman-Kac models (i.e. without any regularity on  $\mathcal{Q}_n$ ). In this setting, (2.13) is satisfied with a r.v.  $\mathbb{X}_n$  with conditional distribution given  $\mathbf{X}_n$  defined by

$$\mathcal{K}_n(\mathbf{X}_n, dx_n) = m(\chi_n)(dx_n) \quad (2.14)$$

**Definition 2.1** *The measures  $(\Pi_n, \Gamma_n)$  and their path space versions  $(\Pi_n, \Gamma_n)$  are called the many body Feynman-Kac measures associated with the particle interpretation (2.3) of the measures  $(\eta_n, \gamma_n)$ .*

As the name ‘‘many-body’’ suggests, these Feynman-Kac models encode properly the collective motion under mean field constraints of the system of particles associated to a standard Feynman-Kac particle system. From an abstract point of view, in view of (2.13), all of these measures are of course essentially equivalent to the abstract Feynman-Kac model introduced in (2.1).



### 3 Conditional particle Markov chain models

This section aims at understanding PMCMC samplers from the point of view of many body Feynman-Kac models.

#### 3.1 Transport equation for many body Feynman-Kac models

We start the section with a pivotal duality formula between the Feynman-Kac integral operators  $(Q_n, \mathcal{Q}_n)$ .

**Lemma 3.1** *We have the duality formula between integral operators on  $\mathcal{S}_n \times \mathcal{S}_n$*

$$\mathcal{Q}_n(x_{n-1}, dx_n) m(x_n)(dx_n) = (m(x_{n-1})Q_n)(dx_n) \mathcal{M}_{x_n, n}(x_{n-1}, dx_n) \quad (3.1)$$

and

$$\eta_0^{\otimes N}(dx_0) m(x_0)(dx_0) = \eta_0(dx_0) \mu_{x_0}(dx_0)$$

with the collection of Markov transitions

$$\mathcal{M}_{x_n, n}(x_{n-1}, dx_n) = \frac{1}{N} \left[ \sum_{i=0}^{N-1} \Phi_n(m(x_{n-1}))^{\otimes(i)} \otimes \delta_{x_n} \otimes \Phi_n(m(x_{n-1}))^{\otimes(N-i-1)} \right] (dx_n)$$

and the distribution

$$\mu_{x_0} := \frac{1}{N} \sum_{i=0}^{N-1} \left( \eta_0^{\otimes(i)} \otimes \delta_{x_0} \otimes \eta_0^{\otimes(N-i-1)} \right)$$

**Proof:**

To check (3.1) we use the symmetry properties of the Markov transitions  $\mathcal{M}_n$  to check that for any function  $H_n \in \mathcal{B}(\mathcal{S}_n \times \mathcal{S}_n)$  (extended by right composition with the canonical projection from  $\mathcal{S}_n^N$  to  $\mathcal{S}_n$  to a function still written  $H_n$  in  $\mathcal{B}(\mathcal{S}_n \times \mathcal{S}_n^N)$ ), we have

$$\begin{aligned} & \int \mathcal{Q}_n(x_{n-1}, dx_n) m(x_n)(dz_n) H_n(z_n, x_n) \\ &= \mathcal{G}_{n-1}(x_{n-1}) \int \Phi_n(m(x_{n-1}))^{\otimes N}(dx_n) H_n(x_n^1, x_n) \\ &= m(x_{n-1})(G_{n-1}) \int \Phi_n(m(x_{n-1}))(dx_n^1) [\delta_{x_n^1} \otimes \Phi_n(m(x_{n-1}))^{\otimes(N-1)}] (dy_n) H_n(x_n^1, y_n) \end{aligned}$$

The end of the proof comes from the fact that

$$m(x_{n-1})(G_{n-1}) \Phi_n(m(x_{n-1}))(dx_n^1) = (m(x_{n-1})Q_n)(dx_n^1)$$

The proof of the lemma is now completed. ■

**Definition 3.2** *Given a random path  $(X_n)_{n \geq 0}$  we let  $\mathcal{X}_n = \{\mathcal{X}_n^i\}_{i=1 \dots N} \in \mathcal{S}_n$  be the Markov chain with the transitions  $\mathcal{M}_{X_n, n}$ , and the initial distribution  $\mu_{X_0}$  introduced in lemma 3.1. We denote by  $\mathbf{M}_n(\mathbf{X}_n, \mathbf{dx}_n)$  the conditional distributions of the random path  $\mathcal{X}_n = (\mathcal{X}_p)_{0 \leq p \leq n}$  on  $\mathcal{S}_n$ . The process  $\mathcal{X}_n$  is called the dual mean field model associated with the Feynman-Kac particle model  $\chi_n$  and the frozen path  $X_n$ .*

The justification of the "duality" terminology between the processes  $\mathcal{X}_n$  and  $\chi_n$  is discussed in the end of the section. The Feynman-Kac measures  $(\gamma_n, \eta_n)$  and their many body version  $(\mathbf{\Gamma}_n, \mathbf{\Pi}_n)$  are connected by the following duality theorem which can be seen as an extended version of the unbiasedness properties (2.13).

**Theorem 3.3** For any  $\mathbf{F}_n \in \mathcal{B}(\mathcal{S}_n)$  by the following equations

$$\mathbb{E} \left( \mathbf{F}_n(\boldsymbol{\chi}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\boldsymbol{\chi}_p) \right) = \mathbb{E} \left( \mathbf{F}_n(\mathbf{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathbf{X}_p) \right) \quad (3.2)$$

When the integral operators  $Q_n$  have some densities  $H_n$  w.r.t. some reference distributions  $v_n$ , for any  $\mathbf{F}_n \in \mathcal{B}(\mathcal{S}_n \times \mathcal{S}_n)$  by the duality formula

$$\mathbb{E} \left( \mathbf{F}_n(\mathbb{X}_n, \boldsymbol{\chi}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\boldsymbol{\chi}_p) \right) = \mathbb{E} \left( \mathbf{F}_n(\mathbf{X}_n, \mathbf{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathbf{X}_p) \right) \quad (3.3)$$

**Proof:**

The proof of (3.2) is a direct consequence of (3.1). Indeed, using this formula, we find that

$$\begin{aligned} \mathcal{Q}_n(x_{n-1}, dx_n) &= \int [m(x_{n-1})Q_n](dz_n) \mathcal{M}_{z_n, n}(x_{n-1}, dx_n) \\ &= \int m(x_{n-1})(dz_{n-1}) Q_n(z_{n-1}, dz_n) \mathcal{M}_{z_n, n}(x_{n-1}, dx_n) \end{aligned}$$

and therefore

$$\begin{aligned} &\mathcal{Q}_{n-1}(x_{n-2}, dx_{n-1}) \mathcal{Q}_n(x_{n-1}, dx_n) \\ &= \int m(x_{n-2})(dz_{n-2}) Q_{n-1}(z_{n-2}, dz_{n-1}) Q_n(z_{n-1}, dz_n) \\ &\quad \times \mathcal{M}_{z_{n-1}, n-1}(x_{n-2}, dx_{n-1}) \mathcal{M}_{z_n, n}(x_{n-1}, dx_n) \end{aligned}$$

Iterating backward in time we prove (3.2). This ends the proof of the first assertion.

The proof of (3.3) is a also direct consequence of (3.1). Indeed, using this formula, we find that

$$\begin{aligned} &\boldsymbol{\Gamma}_n(d\mathbf{x}_n) \prod_{0 \leq p \leq n} m(x_p)(dx_p) \\ &= \left\{ \prod_{0 \leq p < n} m(x_p)(G_p) \right\} \eta_0^{\otimes N}(dx_0) m(x_0)(dx_0) \left\{ \prod_{1 \leq p \leq n} \mathcal{M}_p(x_{p-1}, dx_p) m(x_p)(dx_p) \right\} \\ &= \left\{ \prod_{0 \leq p < n} m(x_p)(G_p) \right\} \left\{ \eta_0(dx_0) \prod_{1 \leq p \leq n} \Phi_p(m(x_{p-1}))(dx_p) \right\} \mathbb{M}_n(\mathbf{x}_n, d\mathbf{x}_n) \\ &= \left\{ \eta_0(dx_0) \prod_{1 \leq p \leq n} m(x_{p-1})(H_p(\cdot, x_p)) v_p(dx_p) \right\} \mathbb{M}_n(\mathbf{x}_n, d\mathbf{x}_n) \end{aligned}$$

The last assertion comes from the fact that

$$m(x_{p-1})(G_{p-1}) \Phi_p(m(x_{p-1}))(d\mathbf{x}_p) = m(x_{p-1})(H_p(\cdot, z_p)) v_p(d\mathbf{x}_p)$$

On the other hand, we have we have

$$\mathcal{K}_n(\mathbf{x}_n, d\mathbf{x}_n) := m(x_n)(dx_n) \prod_{1 \leq p \leq n} \frac{m(x_{p-1})(dx_{p-1}) H_p(x_{p-1}, x_p)}{m(x_{p-1})(H_p(\cdot, x_p))}$$

where  $d\mathbf{x}_n$  stands for an infinitesimal neighborhood of the path  $\mathbf{x}_n = (x_p)_{0 \leq p \leq n} \in \mathcal{S}_n$ . Recalling that

$$Q_p(x_{p-1}, dx_p) = G_p(x_{p-1}) M_p(x_{p-1}, dx_p) = H_p(x_{p-1}, x_p) v_p(dx_p)$$

This implies that

$$\begin{aligned} & \Gamma_n(\mathbf{dx}_n) \mathcal{K}_n(\mathbf{x}_n, \mathbf{dx}_n) \\ &= \left\{ \eta_0(dx_0) \prod_{1 \leq p \leq n} Q_p(x_{p-1}, dx_p) \right\} \mathbb{M}_n(\mathbf{x}_n, \mathbf{dx}_n) = \gamma_n(\mathbf{dx}_n) \mathbb{M}_n(\mathbf{x}_n, \mathbf{dx}_n) \end{aligned}$$

The proof of (3.3) is now completed. This ends the proof of the Theorem.  $\blacksquare$

The following Corollary is a direct consequence of (2.13) and (3.3). It provides an interpretation of the conditional distribution of the dual process  $\mathcal{X}_n$  w.r.t. a given frozen trajectory as a conditional many body Feynman-Kac model w.r.t. a random path  $\mathbb{X}_n$  sampled with the backward distribution (2.12).

**Corollary 3.4** *For any  $F_n \in \mathcal{B}(\mathcal{S}_n)$ , and for  $\eta_n$ -almost every path  $\mathbf{x}_n$  we have*

$$\mathbb{E}(F_n(\mathcal{X}_n) \mid \mathbb{X}_n = \mathbf{x}_n) = \frac{\mathbb{E}\left(F_n(\mathcal{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \mid \mathbb{X}_n = \mathbf{x}_n\right)}{\mathbb{E}\left(\prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \mid \mathbb{X}_n = \mathbf{x}_n\right)} \quad (3.4)$$

We end this section with an analytic description of the duality formulae (3.2) and (3.3) in terms of the conditional distributions  $\mathbb{M}_n$  and  $\mathcal{K}_n$  introduced in definition 3.2 and in (2.12). Using (3.2) we have

$$\forall \mathbf{x}_n \in \mathcal{S}_n \quad \mathbb{M}_n(\mathbf{x}_n, \cdot) \ll \eta_n \mathbb{M}_n = \Pi_n$$

Thus, we can define the dual operator  $\mathbb{M}_{n, \eta_n}^*$  of  $\mathbb{M}_n$  from  $\mathbb{L}_1(\eta_n)$  into  $\mathbb{L}_1(\Pi_n)$  given for any  $f_n \in \mathbb{L}_1(\eta_n)$  by

$$\mathbb{M}_{n, \eta_n}^*(f_n) = \frac{\mathbf{d}(\eta_n, f_n \mathbb{M}_n)}{\mathbf{d}(\eta_n \mathbb{M}_n)} = \frac{\mathbf{d}(\eta_n, f_n \mathbb{M}_n)}{\mathbf{d}\Pi_n} \quad \text{with} \quad \eta_n, f_n(\mathbf{dx}_n) := \eta_n(\mathbf{dx}_n) f_n(\mathbf{x}_n)$$

In addition, for any conjugate integers  $\frac{1}{p} + \frac{1}{q} = 1$ , with  $1 \leq p, q \leq \infty$ , and any pair of functions  $(f_n, F_n) \in (\mathbb{L}_p(\eta_n) \times \mathbb{L}_q(\Pi_n))$  we have

$$\Pi_n \left( F_n \mathbb{M}_{n, \eta_n}^*(f_n) \right) = \eta_n \left( \mathbb{M}_n(F_n) f_n \right) \quad (3.5)$$

These constructions shows that formula (3.3) holds true for general models (i.e. even if the integral operators  $Q_n$  don't have a density) where  $\mathbb{X}_n$  stands for a random path with conditional distribution  $\mathbb{M}_{n, \eta_n}^*(\mathcal{X}_n, \cdot)$  given the historical process  $\mathcal{X}_n$ .

For a more detailed discussion on dual Markov transitions we refer the reader to [16, 45]. In the reverse angle, we have

$$\forall \mathbf{x}_n \in \mathcal{S}_n \quad \mathcal{K}_n(\mathbf{x}_n, \cdot) \ll \Pi_n \mathcal{K}_n = \eta_n$$

Thus (3.3) also implies that  $\mathbb{M}_n$  coincides with the dual operator  $\mathcal{K}_{n, \Pi_n}^*$  of  $\mathcal{K}_n$  from  $\mathbb{L}_1(\Pi_n)$  into  $\mathbb{L}_1(\eta_n)$ ; that is, we have that

$$(3.3) \implies \Pi_n \mathcal{K}_n = \eta_n \implies \eta_n \left( f_n \mathcal{K}_{n, \Pi_n}^*(F_n) \right) = \Pi_n (F_n \mathcal{K}_n(f_n))$$

with

$$\mathcal{K}_{n, \Pi_n}^*(z_n, \mathbf{dx}_n) = \Pi_n(\mathbf{dx}_n) \frac{\mathbf{d}\mathcal{K}_n(\mathbf{x}_n, \cdot)}{\mathbf{d}\Pi_n \mathcal{K}_n}(z_n) = \mathbb{M}_n(z_n, \mathbf{dx}_n) \quad (3.6)$$

These formulations underline the duality between the random paths  $\mathcal{X}_n$  and  $\mathbb{X}_n$  under the Feynman-Kac measures  $\eta_n$  and their many-body version  $\Pi_n$ .

### 3.2 Historical processes

Let us suppose that  $(\eta_n, \gamma_n, \xi_n)$  is the historical version of an auxiliary Feynman-Kac model  $(\gamma'_n, \eta'_n, \xi'_n)$  associated with some potential functions  $G'_n$  and some Markov chain  $X'_n$  transitions  $M'_n$  on some state spaces  $S'_n$ . In this situation, the reference Markov chain of the Feynman-Kac models  $(\eta_n, \gamma_n)$  defined in (2.1) coincides with the historical process  $X_n = (X'_0, \dots, X'_n)$  of the chain  $X'_n$ . We also recall that the particle model  $\mathcal{X}_n := \xi_n$  represents the evolution of the genealogical tree model associated with the particle model  $\mathcal{X}'_n := \xi'_n$ .

The same property holds true at the level of the dual processes. More precisely, the dual mean field model  $\mathcal{X}_n$  associated with pair  $(\xi_n, X_n)$  represents the evolution of the genealogical tree model of the dual particle model  $\mathcal{X}'_n$  associated with the pair  $(\xi'_n, X'_n)$ . To be more precise, we observe that the  $i$ -th path space particle

$$\mathcal{X}_n^i = (\mathcal{X}_{0,n}^i, \mathcal{X}_{1,n}^i, \dots, \mathcal{X}_{n,n}^i) \in S_n := (S'_0 \times \dots \times S'_n)$$

of the particle model  $\mathcal{X}_n$  can be interpreted as the line of ancestors  $\mathcal{X}_{p,n}^i$  of the  $i$ -th individual  $\mathcal{X}_{n,n}^i$  at time  $n$ , at every level  $0 \leq p \leq n$ , with  $1 \leq i \leq N$ . This shows that the particle model  $\mathcal{X}'_n = (\mathcal{X}'_{n,n})_{1 \leq i \leq N}$  coincides with the evolution of the individuals  $\mathcal{X}'_{n,n} = (\mathcal{X}'_{n,n})_{1 \leq i \leq N}$ .

It is also important to observe that the dual process  $\mathcal{X}_n$  is defined in terms of frozen historical paths  $X_n = (X'_0, \dots, X'_n)$ . Therefore, for any function  $F_n \in \mathcal{B}(\mathcal{S}_n)$ , we have the  $\eta_n$ -almost sure conditional expectation formula

$$\mathbb{E}(F_n(\mathcal{X}_n) \mid \mathbf{X}_n) = \mathbb{E}(F_n(\mathcal{X}_n) \mid X_n) := \mathbb{M}_n(F_n)(X_n) \quad (3.7)$$

In the further development of this section, we denote by  $\mathcal{G}'_n$  the potential function of the many-body model associated with the Feynman-Kac model  $(\gamma'_n, \eta'_n, \xi'_n)$ ; that is, we have that  $\mathcal{G}'_n(\mathcal{X}'_n) = m(\mathcal{X}'_n)(G'_n)$ . In this notation, formula (3.2) takes the form

$$\mathbb{E} \left( F_n(\mathcal{X}_n) \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \right) = \mathbb{E} \left( F_n(\mathcal{X}_n) \prod_{0 \leq p < n} G'_p(X'_p) \right) \quad (3.8)$$

Choosing a function  $F_n$  that only depends on the marginal populations we find that

$$\begin{aligned} F_n(\mathcal{X}_0, \dots, \mathcal{X}_n) &:= F_n(\mathcal{X}'_0, \dots, \mathcal{X}'_n) \\ \Rightarrow \mathbb{E} \left( F_n(\mathcal{X}'_n) \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \right) &= \mathbb{E} \left( F_n(\mathcal{X}'_n) \prod_{0 \leq p < n} G'_p(X'_p) \right) \end{aligned}$$

Notice that  $\mathcal{X}'_n$  and  $\mathcal{X}'_n$  are  $\mathcal{S}'_n = \prod_{0 \leq p \leq n} \mathcal{S}'_p$  valued random paths with  $\mathcal{S}'_n := S'^{[N]}$ , for any  $n \geq 0$ .

In much the same way, when the integral operators  $Q'_n$  have some densities  $H'_n$  w.r.t. some reference distributions  $\nu'_n$  on  $S'_n$ , the formula (3.3) takes the following form

$$\mathbb{E} \left( F_n(\mathbb{X}'_n, \mathcal{X}'_n) \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \right) = \mathbb{E} \left( F_n(X_n, \mathcal{X}'_n) \prod_{0 \leq p < n} G'_p(X'_p) \right) \quad (3.9)$$

where  $\mathbb{X}'_n := (\mathbb{X}'_p)_{0 \leq p \leq n}$  stands for a random path pn  $S_n$  with distribution

$$\mathcal{K}'_n(\mathcal{X}'_n, dx_n) := m(\mathcal{X}'_n)(dx'_n) \prod_{1 \leq k \leq n} \mathbb{L}_{k,m}(\mathcal{X}'_{k-1})(x'_k, dx'_{k-1})$$

The following Corollary shows that the transport equations imply an interpretation of mean field particle models with frozen trajectories as conditional many body Feynman-Kac models w.r.t. an random ancestral path  $\mathbb{X}'_n$  of the process  $\mathcal{X}'_n$ .

**Corollary 3.5** For any  $n \geq 0$ ,  $F_n \in \mathcal{B}(\mathcal{S}_n \times S_n)$  we have

$$\mathbb{E} \left( \mathbf{F}_n(\mathcal{X}_{n-1}, \mathbb{X}_n) \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \right) = \mathbb{E} \left( \mathbf{F}_n(\mathcal{X}_{n-1}, X_n) \prod_{0 \leq p < n} G'_p(X'_p) \right) \quad (3.10)$$

where  $\mathbb{X}_n$  stands for a random path with conditional distribution  $m(\mathcal{X}_n)$ , given  $\mathcal{X}_n$ . In addition, for any  $F_n \in \mathcal{B}(\mathcal{S}_n)$  and  $\eta_n$ -almost every  $x_n \in S_n$  we have that

$$\frac{\mathbb{E} \left( F_n(\mathcal{X}_{n-1}) \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \mid \mathbb{X}_n = x_n \right)}{\mathbb{E} \left( \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \mid \mathbb{X}_n = x_n \right)} = \mathbb{E} (F_n(\mathcal{X}_{n-1}) \mid X_n = x_n)$$

**Proof:**

Using (3.3), for any function  $\mathbf{F}_n \in \mathcal{B}(\mathcal{S}_{n-1} \times S_n)$  we check that

$$\begin{aligned} & \mathbb{E} \left( \int m(\mathcal{X}_n)(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \right) \\ &= \mathbb{E} \left( \int \Phi_{n-1}(m(\mathcal{X}_{n-1}))(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \right) \\ &= \mathbb{E} \left( \int \Phi_{n-1}(m(\mathcal{X}_{n-1}))(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} G_p(\mathbf{X}_p) \right) \\ &= \mathbb{E} \left( \int m(\mathcal{X}_n)(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} G_p(\mathbf{X}_p) \right) \end{aligned}$$

On the other hand, we have

$$\begin{aligned} & \mathbb{E} \left( \int m(\mathcal{X}_n)(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} G_p(\mathbf{X}_p) \right) \\ &= \frac{1}{N} \mathbb{E} \left( \mathbf{F}_n(\mathcal{X}_{n-1}, X_n) \prod_{0 \leq p < n} G_p(\mathbf{X}_p) \right) \\ &\quad + \left(1 - \frac{1}{N}\right) \mathbb{E} \left( \int \Phi_n(m(\mathcal{X}_{n-1}))(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} G_p(\mathbf{X}_p) \right) \end{aligned}$$

This implies that

$$\mathbb{E} \left( \int m(\mathcal{X}_n)(dx_n) \mathbf{F}_n(\mathcal{X}_{n-1}, x_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \right) = \mathbb{E} \left( \mathbf{F}_n(\mathcal{X}_{n-1}, X_n) \prod_{0 \leq p < n} G_p(X_p) \right)$$

The end of the proof of (3.10) is now clear.  $\blacksquare$

The next result provides a new interpretation of the backward Markov transition  $\mathcal{K}'_n$  in terms of the conditional distribution of a genealogical line given the complete ancestral tree.

**Corollary 3.6** When the integral operators  $Q'_n$  have some densities  $H'_n$  w.r.t. some reference distributions  $v'_n$  on  $S'_n$ , we have

$$\mathbb{E} \left( F_n(\mathcal{X}'_{n-1}, \mathbb{X}_n) \right) = \mathbb{E} \left( F_n(\mathcal{X}'_{n-1}, \mathbb{X}'_n) \right) \quad (3.11)$$

with the random paths  $\mathbb{X}_n$  and  $\mathbb{X}'_n$  on  $S_n$  defined in (3.10) and (3.9). In particular, for any  $f_n \in \mathcal{B}(S_n)$  this implies that

$$\begin{aligned} & \mathbb{E} \left( m(\mathcal{X}_n)(f_n) \mid \mathcal{X}'_{n-1} \right) \\ &= \int \Phi_n(m(\mathcal{X}'_{n-1}))(dx'_n) \left\{ \prod_{1 \leq k \leq n} \mathbb{L}_{k,m}(\mathcal{X}'_{k-1})(x'_k, dx'_{k-1}) \right\} f_n(x'_0, \dots, x'_n) \end{aligned}$$

**Proof:**

Using (3.10) we have

$$\mathbb{E} \left( \int m(\chi_n)(dx_n) F_n(\mathcal{X}'_{n-1}, x_n) \right) = \mathbb{E} \left( F_n(\mathcal{X}'_{n-1}, X_n) \prod_{0 \leq p < n} (G_p(X_p)/\mathcal{G}'_p(\mathcal{X}'_p)) \right)$$

On the other hand, using (3.9) we also have that

$$\mathbb{E} \left( F_n(\mathcal{X}'_{n-1}, \mathbb{X}'_n) \right) = \mathbb{E} \left( F_n(\mathcal{X}'_{n-1}, X_n) \prod_{0 \leq p < n} (G_p(X_p)/\mathcal{G}'_p(\mathcal{X}'_p)) \right)$$

This clearly ends the proof of the Corollary. ■

### 3.3 Genealogy and backward sampling models

**Definition 3.7** *When the integral operators  $Q_n$  have some densities  $H_n$  w.r.t. some distributions  $v_n$ , we consider the Markov transition from  $\mathcal{S}_n$  into itself defined by  $\mathbb{K}_n := \mathbb{M}_n \mathcal{K}_n$ , with the couple of operators  $(\mathbb{M}_n, \mathcal{K}_n)$  introduced in definition 3.2 and in (2.12).*

*When  $(\eta_n, \gamma_n)$  is the historical version of an auxiliary Feynman-Kac model  $(\gamma'_n, \eta'_n)$ , we consider the Markov transition from  $S_n$  into itself defined by  $\mathbb{K}_n := \mathbb{M}_n \mathcal{K}_n$ , with the couple of operators  $(\mathbb{M}_n, \mathcal{K}_n)$  introduced in (3.7) and in (2.14).*

**Proposition 3.8** *The Markov transitions  $\mathbb{K}_n$ , resp.  $\mathbb{K}_n$  are reversible w.r.t. the probability measures  $\eta_n$ , resp.  $\eta_n$*

Three elementary proofs of these regularity properties can be underlined:

- Using (3.3), for any couple of functions  $f_1, f_2 \in \mathcal{B}(\mathcal{S}_n)$  we have

$$\begin{aligned} & \mathbb{E} \left( \mathcal{K}_n(f_1)(\mathcal{X}_n) \mathcal{K}_n(f_2)(\mathcal{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \right) \\ &= \mathbb{E} \left( f_1(\mathbb{X}_n) \mathcal{K}_n(f_2)(\mathcal{X}_n) \prod_{0 \leq p < n} \mathcal{G}_p(\mathcal{X}_p) \right) \propto \mathbb{E} (f_1(\mathbf{X}_n) \mathbb{K}_n(f_2)(\mathbf{X}_n)) \end{aligned}$$

Recalling that  $\mathcal{K}_n(x_n, \cdot)$  and  $\mathbb{K}_n(x_n, \cdot)$  are the  $S_n$ -marginal of the measures  $\mathcal{K}_n(x_n, \cdot)$  and  $\mathbb{K}_n(x_n, \cdot)$ , (for any  $\eta_n$ -p.s., trajectory  $\mathbf{x}_n = (x_p)_{0 \leq p \leq n} \in \mathcal{S}_n$ ), for any  $(f_1, f_2) \in \mathcal{B}(S_n)^2$  the above result implies that

$$\mathbb{E} \left( m(\mathcal{X}_n)(f_1) m(\mathcal{X}_n)(f_2) \prod_{0 \leq p < n} \mathcal{G}'_p(\mathcal{X}'_p) \right) \propto \mathbb{E} (f_1(X_n) \mathbb{K}_n(f_2)(X_n))$$

By symmetry arguments the reversibility follows.

- Combining the unbiasedness properties of the unnormalized particle measures  $\gamma_n^{(N,2)}$  with the transport equation (3.2) we have

$$(\eta_n = \mathbb{M}_n \mathcal{K}_n \quad \text{and} \quad \mathbb{M}_n = \eta_n \mathbb{M}_n) \implies \eta_n = \eta_n \mathbb{M}_n \mathcal{K}_n = \eta_n \mathbb{K}_n$$

In much the same way, using the unbiasedness properties of the unnormalized particle measures  $\gamma_n^{(N,1)}$  we check that

$$(\eta_n = \mathbb{M}_n \mathcal{K}_n \quad \text{and} \quad \mathbb{M}_n = \eta_n \mathbb{M}_n) \implies \eta_n = \eta_n \mathbb{M}_n \mathcal{K}_n = \eta_n \mathbb{K}_n$$

- The reversibility of  $\mathbb{K}_n = \mathcal{K}_{n, \Pi_n}^* \mathcal{K}_n$  is also a direct consequence of the the duality formula (3.5). Indeed, for any  $(\mathbf{f}_1, \mathbf{f}_2) \in \mathbb{L}_2(\eta_n)^2$  we have that

$$(3.6) \Rightarrow \eta_n(\mathbf{f}_1 \mathbb{K}_n(\mathbf{f}_2)) = \Pi_n(\mathcal{K}_n(\mathbf{f}_1) \mathcal{K}_n(\mathbf{f}_2)) = \eta_n(\mathbb{K}_n(\mathbf{f}_1) \mathbf{f}_2) \quad (3.12)$$

Since  $\mathbb{K}_n(x_n, \cdot)$  is the  $S_n$ -marginal of the measures  $\mathbb{K}_n(\mathbf{x}_n, \cdot)$ , we also have

$$(3.12) \implies \forall (f_1, f_2) \in \mathbb{L}_2(\eta_n)^2 \quad \eta_n(\mathbb{K}_n(f_1) f_2) = \eta_n(f_1 \mathbb{K}_n(f_2))$$

Next, we present an elementary proof of the ergodicity of the couple of conditional PMCMC transitions discussed above. Sharp estimates of the contraction properties of  $\mathbb{K}_n$  and *its iterates*  $\mathbb{K}_n^m$ , with  $m \geq 1$ , are developed in section 3.4. These quantitative estimates are based on new Taylor type expansions of the PMCMC transitions around the limiting invariant measure  $\eta_n$  w.r.t. the precision parameter  $1/N$ .

**Proposition 3.9** *The measure  $\eta_n$  and  $\eta_n$  are the unique invariant measures of the Markov transitions  $\mathbb{K}_n$  and  $\mathbb{K}_n$ . In addition, we have the estimates*

$$\beta(\mathbb{K}_n) \vee \beta(\mathbb{K}_n) \leq 1 - \tau_n \left(1 - \frac{1}{N}\right)^{n+1} \quad \text{for some } \tau_n \geq \prod_{0 \leq p < n} g_p \quad (3.13)$$

The estimates (3.13) are direct consequence of the following rather crude uniform estimate

$$\mathbb{K}_n(\mathbf{f}_n)(\mathbf{x}_n) \geq \tau_n \left(1 - \frac{1}{N}\right)^{n+1} \eta_n(\mathbf{f}_n)$$

for any non negative function  $\mathbf{f}_n$  on  $\mathbf{S}_n$ , and any path sequence  $\mathbf{z}_n = (z_p)_{0 \leq p \leq n}$ . These lower bounds are easily checked by induction w.r.t. the time parameter. By construction, for any  $\mathbf{z}_n = (\mathbf{z}_{n-1}, z_n) \in \mathbf{S}_n = (\mathbf{S}_{n-1} \times S_n)$  we have

$$\mathbb{K}_n(\mathbf{f}_n)(\mathbf{z}_n) \geq \left(1 - \frac{1}{N}\right) g_{n-1} \mathbb{K}_{n-1}(\overline{\mathcal{Q}}_n(\mathbf{f}_n))(\mathbf{z}_{n-1})$$

with the integral operators  $\overline{\mathcal{Q}}_n$  defined as  $\overline{\mathcal{Q}}_n$  by replacing  $(G_n, M_n, \eta_n)$  by  $(\mathbf{G}_n, \mathbf{M}_n, \eta_n)$ . Iterating these estimates we check (3.13). We can alternatively use the fact that

$$\begin{aligned} & \tau_n^{-1} \mathbb{K}_n(\mathbf{f}_n)(\mathbf{x}_n) \\ & \geq \mathbb{E} \left( \left\{ \prod_{0 \leq p < n} m(\mathcal{X}_p)(\overline{\mathcal{G}}_p) \right\} \mathcal{K}_n(\mathbf{f}_n)(\mathcal{X}_n) \mid \mathbf{X}_n = \mathbf{x}_n \right) \geq \left(1 - \frac{1}{N}\right)^{n+1} \eta_n(\mathbf{f}_n) \end{aligned}$$

### 3.4 Taylor type expansions around the invariant measure

We assume in this paragraph that  $(\eta_n, \gamma_n, \xi_n)$  is the historical version of an auxiliary Feynman-Kac model  $(\gamma'_n, \eta'_n, \xi'_n)$ . Our first objective is to find a Taylor type expansion of the Markov transition  $\mathbb{K}_n$  around its invariant measure  $\eta_n$  w.r.t. powers of  $1/N$ . We fix the time horizon  $n$  and a frozen trajectory  $z_n := (z'_0, \dots, z'_n) \in S_n = (S'_0 \times \dots \times S'_n)$ , and for any  $0 \leq p \leq n$  we set  $z_p := (z'_0, \dots, z'_p) \in S_p$ .

We denote by  $\mathcal{X}_{z_n, n}$  the dual mean field model associated with the Feynman-Kac particle model  $\mathcal{X}_n$  and the frozen path  $X_n = z_n$ . Using the exchangeability properties of the dual particles, there is no loss of generality to assume that only the first one  $\mathcal{X}_{z_n, n}^1 = X_n$  is frozen. With this convention, for any function  $f_n \in \mathcal{B}(S_n)$  we have

$$\mathbb{K}_n(f_n)(z_n) = \mathbb{E}(m(\mathcal{X}_{z_n, n})(f_n)) = \frac{1}{N} f_n(z_n) + \left(1 - \frac{1}{N}\right) \mathbb{E}(m(\mathcal{X}_{z_n, n}^-(f_n)))$$

where  $m(\mathcal{X}_{z_n,n}^-)$  stands for the occupation measure of the non frozen particles  $m(\mathcal{X}_{z_n,n}^-) := \frac{1}{N-1} \sum_{1 < i \leq N} \delta_{\mathcal{X}_{z_n,n}^i}$ . This shows that whenever they exists these Taylor expansions are related to the bias and the fluctuations of the measures  $m(\mathcal{X}_{z_n,n}^-)$ . To analyze these properties we observe that

$$\mathbb{E} \left( m(\mathcal{X}_{z_n,n})(f_n) \mid \mathcal{X}_{z_{n-1},n-1} \right) = \Phi_{z_n,n} \left( m(\mathcal{X}_{z_{n-1},n-1}) \right) (f_n)$$

with the one step transformations  $\Phi_{z_n,n}$  defined as  $\Phi_n$  by replacing the Markov transitions  $M_n$  by

$$M_{z_n,n}(x_{n-1}, dx_n) = \frac{1}{N} \delta_{z_n}(dx_n) + \left( 1 - \frac{1}{N} \right) M_n(x_{n-1}, dx_n)$$

In addition, the occupation measures  $m(\mathcal{X}_{z_n,n}^-)$  of all the particles but the first frozen ones are based on  $(N-1)$  conditionally independent random states with common law  $\Phi_n(m(\mathcal{X}_{z_{n-1},n-1}))$ . Thus, the local fluctuations of  $m(\mathcal{X}_{z_n,n})$  around  $\Phi_{z_n,n}(m(\mathcal{X}_{z_{n-1},n-1}))$  can be expressed in terms of the local sampling random fields

$$V_n^N := \sqrt{N-1} \left[ m(\mathcal{X}_{z_n,n}^-) - \Phi_n(m(\mathcal{X}_{z_{n-1},n-1})) \right]$$

with the formula

$$m(\mathcal{X}_{z_n,n})(f_n) = \Phi_{z_n,n} \left( m(\mathcal{X}_{z_{n-1},n-1}) \right) + \left( 1 - \frac{1}{N} \right) \frac{1}{\sqrt{N-1}} V_n^N$$

**Proposition 3.10** *Let  $X_{z_n,n}$  stand for a Markov chain on  $S_n$ , with initial distribution  $\eta_{z_0,0} = \frac{1}{N} \delta_{z_0} + (1 - \frac{1}{N}) \eta_0$  and Markov transitions  $M_{z_n,n}$  from  $S_{n-1}$  into  $S_n$ . We have*

$$\mathbb{E} \left( m(\mathcal{X}_{z_n,n})(f_n) \prod_{0 \leq p < n} m(\mathcal{X}_{z_p,p})(G_p) \right) = \mathbb{E} \left( f_n(X_{z_n,n}) \prod_{0 \leq p < n} G_p(X_{z_p,p}) \right) \quad (3.14)$$

The proof is similar to the one that  $\gamma_n^{(N,1)}$  is an unbiased approximation of  $\gamma_n$  and omitted, see [15].

The r.h.s. Feynman-Kac measure in (3.14) can be expressed in terms of powers of the precision parameter  $1/N$ . To describe these models, we let  $\epsilon_n$  be a sequence of independent  $\{0,1\}$ -valued random variables with  $\mathbb{P}(\epsilon_n = 1) = 1/N$ . For any  $\epsilon = (\epsilon_p)_{0 \leq p \leq n} \in \{0,1\}^{n+1}$  we set  $X_{z_n,n}^{(\epsilon)}$  be a Markov chain on  $S_n$ , with initial distribution  $\eta_{z_0,0}^{(\epsilon)}$  and Markov transitions  $M_{z_n,n}^{(\epsilon)}$  defined by

$$\begin{aligned} \eta_{z_0,0}^{(\epsilon)} &= \epsilon_0 \delta_{z_0} + (1 - \epsilon) \eta_0 \\ M_{z_n,n}^{(\epsilon)}(x_{n-1}, dx_n) &= \epsilon_n \delta_{z_n}(dx_n) + (1 - \epsilon_n) M_n(x_{n-1}, dx_n) \end{aligned}$$

In this notation, we readily check that

$$\begin{aligned} \mathbb{E} \left( f_n(X_{z_n,n}) \prod_{0 \leq p < n} G_p(X_{z_p,p}) \right) &= \left( 1 - \frac{1}{N} \right)^{(n+1)} \gamma_n(f_n) \\ &+ \sum_{1 \leq p \leq n+1} \left( \frac{1}{N} \right)^p \left( 1 - \frac{1}{N} \right)^{(n+1)-p} \sum_{\epsilon_0 + \dots + \epsilon_n = p} \mathbb{E} \left[ f_n(X_{z_n,n}^{(\epsilon)}) \prod_{0 \leq p < n} G_p(X_{z_p,p}^{(\epsilon)}) \right] \end{aligned}$$

These decompositions can be easily turned into Taylor's type polynomial expansions in power of  $1/N$ . The Taylor expansion of the normalized Feynman-Kac measures with the 0-th order measure  $\eta_n$  follows standard arguments on quotient power series.

The next proposition is easily proved using rather standard stochastic perturbation techniques (cf. for instance [15, 21]).



**Proposition 3.11** *The random fields  $\sqrt{N}[m(\mathcal{X}_{z_n,n}) - \eta_n]$  and  $\sqrt{N}[m(\xi_n) - \eta_n]$  converge in law as  $N \uparrow \infty$  to the same Gaussian and centered random fields. The same property holds true for the random fields associated with the unnormalized particle measures. In addition, for any function  $f_n \in \mathcal{B}(S_n)$  s.t.  $\eta_n(f_n) = 0$ , and any frozen trajectory  $z_n = (z'_p)_{0 \leq p \leq n} \in S_n = \prod_{0 \leq p \leq n} S'_p$  we have the asymptotic bias expansion*

$$\lim_{N \uparrow \infty} N \mathbb{K}_n(f_n)(z_n) = \sum_{0 \leq p \leq n} \eta_p \left( \overline{\mathcal{Q}}_{p,n}(1) \left[ \overline{\mathcal{Q}}_{p,n}(f_n)(z_p) - \overline{\mathcal{Q}}_{p,n}(f_n) \right] \right) \quad (3.15)$$

with  $z_p := (z'_0, \dots, z'_p) \in S_p$ , for any  $p \leq n$ .

To get one step further, we need to analyze the propagation properties of the non frozen particles.

**Theorem 3.12** *For any  $N > 1$ ,  $n \geq 0$ , and any order  $l < \lfloor (N-1)/2 \rfloor$  we have the Taylor expansion*

$$\mathbb{K}_n(z_n, dy_n) = \eta_n(dy_n) + \sum_{1 \leq k \leq l} \frac{1}{N^k} d^{(k)} \mathbb{K}_n(z_n, dy_n) + \mathcal{O}\left(\frac{1}{N^{l+1}}\right) \quad (3.16)$$

for some sequence of signed and bounded integral operators  $d^{(k)} \mathbb{K}_n$  s.t.

$$\forall k \geq 1 \quad d^{(k)} \mathbb{K}_n(1)(z_n) = 0 \quad \text{and} \quad \int \eta_n(dz_n) d^{(k)} \mathbb{K}_n(z_n, dy_n) f_n(y_n) = 0 \quad (3.17)$$

for any function  $f_n$  on the path space  $S_n$ .

This Theorem is a particular case of the more general Theorem 4.21, that can basically be stated as follows. We let

$$\mathbb{P}_{z_n,n}^{(N,q)} = \text{Law} \left( \mathcal{X}_{z_n,n}^2, \mathcal{X}_{z_n,n}^3, \dots, \mathcal{X}_{z_n,n}^{q+1} \right) \quad (3.18)$$

be the distribution of the first  $q$  random non frozen particles  $\mathcal{X}_{z_n,n}^{i+1}$   $i = 1, \dots, q$ . In this notation, for any  $1 \leq q \leq N$ ,  $N > 1$ ,  $n \geq 0$ , and any order  $l < \lfloor (N-q)/2 \rfloor$  we have the Taylor expansion

$$\mathbb{P}_{z_n,n}^{(N,q)} = \eta_n^{\otimes q} + \sum_{1 \leq k \leq l} \frac{1}{N^k} d^{(k)} \mathbb{P}_{z_n,n}^{(q)} + \mathcal{O}\left(\frac{1}{N^{l+1}}\right) \quad (3.19)$$

for some signed and bounded measures  $d^{(k)} \mathbb{P}_{z_n,n}^{(q)}$  with null mass  $d^{(k)} \mathbb{P}_{z_n,n}^{(q)}(1) = 0$  whose values don't depend on the population size  $N$ .

We end this section with some direct consequences of these expansions around the fixed point Feynman-Kac measures.

- These expansions can also be used to estimate of the behavior of the particle measures  $m(\xi_{z_n,n})$  as  $N \uparrow \infty$ . For instance, we have the bias and the variance estimates

$$\mathbb{E}(m(\mathcal{X}_{z_n,n})(f_n)) = \eta_n(f_n) + \frac{1}{N} \left( [f_n(z_n) - \eta_n(f)] + d^{(1)} \mathbb{P}_{z_n,n}^{(1)}(f) \right) + \mathcal{O}\left(\frac{1}{N^2}\right)$$

and

$$\text{Var}(m(\mathcal{X}_{z_n,n})(f_n)) = \frac{1}{N} [\eta_n(f_n^2) - \eta_n(f_n)^2] + \mathcal{O}\left(\frac{1}{N^2}\right)$$

The last estimate is related to the variance of the particle measures  $m(\mathcal{X}_{z_n,n})$  delivered by the PMCMC model. In much the same way, the variance of a function of the trajectory delivered by the PMCMC model is computed using the expansion of  $\mathbb{E}(m(\mathcal{X}_{z_n,n})(f_n^2))$ .

- Using the first order expansion (3.16), for any  $\mu_n, \nu_n \in \mathcal{P}(S_n)$  we readily check that

$$(\mu_n - \nu_n) \mathbb{K}_n = \frac{1}{N} (\mu_n - \nu_n) d^{(1)} \mathbb{K}_n + \mathcal{O}\left(\frac{1}{N^2}\right)$$

with the first order integral operator  $d^{(1)}\mathbb{K}_n$  defined in (3.15) and given by

$$d^{(1)}\mathbb{K}_n(f_n)(z_n) = \sum_{0 \leq p \leq n} \eta_p(\bar{Q}_{p,n}(1)) [\bar{Q}_{p,n}(f_n)(z_p) - \bar{Q}_{p,n}(f_n)]$$

This implies that

$$\beta(\mathbb{K}_n) = \frac{1}{N} \beta(d^{(1)}\mathbb{K}_n) + O\left(\frac{1}{N^2}\right)$$

Using (3.15), we also have the crude estimate

$$\beta(d^{(1)}\mathbb{K}_n) \leq 2 \sum_{0 \leq k \leq n} \|\bar{Q}_{k,n}(1)\|$$

The r.h.s. term can be estimated using well known Feynman-Kac semigroup techniques. For instance, using the estimate (12.9) in lemma 12.2.2 in [21], we have the uniform estimate  $\sup_{k \leq n} \|\bar{Q}_{k,n}(1)\| \leq c$  for some finite constant  $c < \infty$  as soon as the semigroup  $\Phi'_{k,n}(\eta'_k) = \eta'_n$  of the  $n$ -th time marginal measures  $\eta'_n$  forgets exponentially fast its initial condition. In this case, the summation term in the r.h.s. of the above displayed formula grows linearly w.r.t. the time horizon and the function  $O(N^{-2})$  can be replaced by  $O\left(\frac{1}{(n/N)^2}\right)$ . These estimates ensures that the Markov chain with transitions  $\mathbb{K}_n$  converge exponentially fast to  $\eta_n$  with a rate that can be made arbitrary large when the precision parameter and the size of the particle population model  $N \uparrow \infty$ .

• Using the properties (3.17) we readily prove Taylor expansions of any  $m$ -th iterate  $\mathbb{K}_n^m = \mathbb{K}_n^{m-1}\mathbb{K}_n$  of the PMCMC transition  $\mathbb{K}_n$ . More precisely, for any  $m \geq 1$ , we have

$$\mathbb{K}_n^m(y_n, dz_n) = \eta_n(dz_n) + \frac{1}{N^m} \left[ \sum_{0 \leq k \leq l} \frac{1}{N^k} d^{(m+k)}\mathbb{K}_n^m(y_n, dz_n) + O\left(\frac{1}{N^{l+1}}\right) \right] \quad (3.20)$$

with the  $(m+k)$ -th order derivative

$$d^{(m+k)}\mathbb{K}_n^m = \sum_{k_1 + \dots + k_m = k} d^{(k_1+1)}\mathbb{K}_n \dots d^{(k_m+1)}\mathbb{K}_n$$

In the above display the summation is taken over all integers  $k_l \geq 0$ , with  $1 \leq l \leq m$ . This result shows that the distribution of the random state of the Markov chain with transition  $\mathbb{K}_n$  after  $m$  iteration is equal to  $\eta_n$  up to some remainder measure with total variation norm of order  $N^{-m}$ . In addition, arguing as above we find that

$$\beta(\mathbb{K}_n^m) = \frac{1}{N^m} \beta\left(\left[d^{(1)}\mathbb{K}_n\right]^m\right) + O\left(\frac{1}{N^{m+1}}\right)$$

with the  $m$ -th iterate  $\left[d^{(1)}\mathbb{K}_n\right]^m := \left[d^{(1)}\mathbb{K}_n\right]^{m-1} d^{(1)}\mathbb{K}_n$  of the operator  $d^{(1)}\mathbb{K}_n$ .

• The decompositions (3.20) can be used to derive without any additional work the  $\mathbb{L}_p$ -norms between the distributions of the random states of the conditional PMCMC model and the invariant measures. For instance, for any  $p \geq 1$  we have

$$\|\mathbb{K}_n^m(f_n) - \eta_n\|_{\mathbb{L}_p(\eta_n)} = \frac{1}{N^m} \left\| \left[ d^{(1)}\mathbb{K}_n \right]^m(f_n) \right\|_{\mathbb{L}_p(\eta_n)} + O\left(\frac{1}{N^{m+1}}\right)$$

• The proof of the Taylor expansions (3.18) is based on renormalization techniques and a differential calculus on the measures  $\Upsilon_{z_n, n}^{(N, q)}$  on  $S_n^q$  defined for any  $F_n \in \mathcal{B}(S_n^q)$  by

$$\Upsilon_{z_n, n}^{(N, q)}(F_n) := \mathbb{E} \left( m(\mathcal{X}_{z_n, n})^{\otimes q}(F_n) \prod_{0 \leq p < n} m(\mathcal{X}_{z_p, p})(\bar{G}_p)^q \right) \quad (3.21)$$

We will show that  $\Upsilon_{z_n, n}^{(N, q)}$  are differentiable at any order with  $d^{(0)}\Upsilon_{z_n, n}^{(N, q)} = \eta_n^{\otimes q}$ . On the other hand, formula (3.2) implies that

$$\int \eta_n(dz_n) \Upsilon_{z_n, n}^{(N, q-1)}(F_n) = \Upsilon_n^{(N, q)}(F_n \otimes 1) \quad (3.22)$$

for any  $F_n \in \mathcal{B}(S_n^{q-1})$ , with the measure  $\Upsilon_n^{(N, q)}$  defined as  $\Upsilon_{z_n, n}^{(N, q)}$  by replacing  $(\mathcal{X}_{z_p, p})_{0 \leq p \leq n}$  by  $(\mathcal{X}_n)_{0 \leq p \leq n}$ . This formula can be used to compute Taylor type expansions for the occupation measures of the process  $\mathcal{X}_n$ , including the  $(q+1)$ -moments of the unnormalized particle normalizing constants  $\prod_{0 \leq p < n} m(\mathcal{X}_p)(G_p)$ .

In this connexion, the transfer formula (3.22) also shows that the particle approximation  $\prod_{0 \leq p < n} m(\mathcal{X}_p)(G_p)$  of the normalizing constants associated with the particle model with a frozen trajectory is *biased even if the particle Markov chain model starts with the desired target measure*. For instance for  $q = 1$  and  $F_n = 1$  formula (3.22) implies that

$$\mathbb{E} \left( \prod_{0 \leq p < n} m(\mathcal{X}_p)(\overline{G}_p) \right) = 1 + \mathbb{E} \left( \left[ \prod_{0 \leq p < n} m(\mathcal{X}_p)(\overline{G}_p) - 1 \right]^2 \right) \neq 1$$

Running a Markov chain with one of the transitions  $\mathbb{K}_n$ , we design a asymptotically unbiased estimate using the easily checked formula

$$\mathbb{E} \left( \left[ \prod_{0 \leq p < n} m(\mathcal{X}_p)(G_p) \right]^{-1} \right) = \left[ \prod_{0 \leq p < n} \eta_p(G_p) \right]^{-1}$$

## 4 Propagation of chaos expansions

This section, as its name indicates, will focus on the fine analysis of the size  $N$  dependency of PMCMC samplers and related problems such as asymptotic independency of  $q \ll N$  subsets of the particle models investigated in the first sections of the article –that is, propagation of chaos properties.

### 4.1 Combinatorial preliminaries

We let  $X = (X^i)_{2 \leq i \leq N}$  be a sequence of random variables on some state space  $S$ , and  $z \in S$  a given fixed state. For any  $q < N$  we set

$$m(X)^{\odot q} = \frac{1}{(N-1)_q} \sum_{a \in I_q^N} \delta_{(X^{a(1)}, \dots, X^{a(q)})}$$

where  $I_q^N$  stands the set of all  $(N-1)_q = \frac{(N-1)!}{((N-1)-q)!}$  multi-indexes  $a = (a(1), \dots, a(q)) \in \{2, \dots, N\}^q$  with different values, or equivalently one to one mappings from  $[q] := \{1, \dots, q\}$  into  $\{2, \dots, N\} = [N] - \{1\}$ . The link between these measures and tensor product measures is expressed in terms of the Markov transitions  $\mathbb{A}_a^{(q)}$  indexed by the set of mappings  $a$  from  $[q]$  into itself and defined for any  $x = (x^1, \dots, x^q) \in S^q$  by

$$\mathbb{A}_a^{(q)}(F)(x) = F(x^a) \quad \text{with} \quad x^a := (x^{a(1)}, \dots, x^{a(q)})$$

for any function  $F$  on  $\mathcal{B}(S^q)$ , and any  $(x^1, \dots, x^q) \in S^q$ . The connection between these measures is described in the following technical lemma taken from [22].

We emphasize that the tensor product measures discussed above are symmetry-invariant by construction. In the further development of this section, it is assumed without restrictions that these measures act on symmetric functions  $F$ ; that is  $F = \frac{1}{q!} \sum_{\sigma \in \mathcal{G}_q} \mathbb{A}_\sigma^{(q)}(F)$ , where  $\mathcal{G}_q$  stands for the symmetric group of all permutations of  $[q]$ .

**Lemma 4.1** For any  $q < N$  we have the formula

$$m(X)^{\otimes q} = m(X)^{\odot q} \mathbb{A}^{(N,q)} \quad \text{with} \quad \mathbb{A}^{(N,q)} = \frac{1}{(N-1)^q} \sum_{a \in [q]^{[q]}} \frac{(N-1)^{|a|}}{(q)^{|a|}} \mathbb{A}_a^{(q)}$$

where  $|a|$  for the cardinality of the set  $a([q])$ , and  $(m)_p = m!/(m-p)!$  stands for the number of one to one mappings from  $[p]$  into  $[m]$ .

**Definition 4.2** For any  $z \in S$  we consider the random measures

$$m_z(X) = \frac{1}{N} \delta_z + \left(1 - \frac{1}{N}\right) m(X) \quad m_z^{(1)}(X) = \delta_z \quad \text{and} \quad m_z^{(0)}(X) = m(X)$$

For any  $b \in \{0, 1\}^{[q]}$ , we denote by  $\mathbb{B}_{z,b}^{(q)}$  the Markov transitions defined for any  $x = (x^1, \dots, x^q) \in S^q$  by

$$\mathbb{B}_{z,b}^{(q)}(F)(x) = F\left(x_z^b\right) \quad \text{with} \quad x_z^b := (b(1)z + (1-b(1))x^1, \dots, b(q)z + (1-b(q))x^q)$$

We observe that

$$m_z(X)^{\otimes q} = \sum_{b \in \{0,1\}^{[q]}} \frac{1}{N^{|b|_1}} \left(1 - \frac{1}{N}\right)^{q-|b|_1} m_z^{(b)}(X)$$

with  $|b|_1 = \sum_{1 \leq p \leq q} b(p)$  and

$$m_z^{(b)}(X) = m_z^{(b(1))}(X) \otimes \dots \otimes m_z^{(b(q))}(X)$$

**Lemma 4.3** For any  $q < N$ , and  $b \in \{0, 1\}^{[q]}$  we have  $m_z^{(b)}(X) = m^{\otimes q}(X) \mathbb{B}_{z,b}^{(N,q)}$  and

$$m_z(X)^{\otimes q} = m^{\otimes q}(X) \mathbb{B}_z^{(N,q)} \quad \text{with} \quad \mathbb{B}_z^{(N,q)} = \sum_{b \in \{0,1\}^{[q]}} \frac{1}{N^{|b|_1}} \left(1 - \frac{1}{N}\right)^{q-|b|_1} \mathbb{B}_{z,b}^{(q)}$$

as well as

$$m_z(X)^{\otimes q} = m(X)^{\odot q} \mathbb{C}_z^{(N,q)} \quad \text{with} \quad \mathbb{C}_z^{(N,q)} := \mathbb{A}^{(N,q)} \mathbb{B}_z^{(N,q)}$$

**Definition 4.4** We let  $(p_1, p_2)$  be a couple of integers s.t.  $0 \leq p_1 \leq q-1$  and  $0 \leq p_2 \leq q$ .

- We consider the collection of sets

$$\begin{aligned} \mathcal{I}_q &:= \{0, \dots, q-1\} \times \{0, \dots, q\} & [r]_{q-p_1}^{[q]} &:= \{a \in [r]^{[q]} : |a| = q-p_1\} \\ \{0, 1\}_{1,p_2}^{[q]} &:= \{b \in \{0, 1\}^{[q]} : |b|_1 = p_2\} & \text{and} & I_q(p_1, p_2) = [q]_{q-p_1}^{[q]} \times \{0, 1\}_{1,p_2}^{[q]} \end{aligned}$$

- We let  $\mathcal{A}_{p_1}^{(q)}$ , and resp.  $\mathcal{B}_{p_2}^{(q)}$  be the uniform distributions on  $[q]_{q-p_1}^{[q]}$ , and resp. on  $\{0, 1\}_{1,p_2}^{[q]}$ . We also denote by  $\mathcal{C}_{p_1, p_2}^{(q)} = \mathcal{A}_{p_1}^{(q)} \otimes \mathcal{B}_{p_2}^{(q)}$  the uniform measure on  $I_q(p_1, p_2)$ .
- For any  $c = (a, b) \in I_q(p_1, p_2)$ , we let  $\mathbb{C}_{z,(a,b)}^{(q)}$  be the coalescent operator defined for any  $x = (x^1, \dots, x^q) \in S^q$  by

$$\mathbb{C}_{z,(a,b)}^{(q)}(F)(x) := F(x_z^{(a,b)})$$

with

$$x_z^{(a,b)} = \left(b(1)z + (1-b(1))x^{a(1)}, \dots, b(q)z + (1-b(q))x^{a(q)}\right),$$

so that  $\mathbb{C}_{z,(a,b)}^{(q)} = \mathbb{A}_a^{(q)} \mathbb{B}_{z,b}^{(q)}$ .

**Remark 4.5** When maps in  $[q]^{[q]}$  are represented graphically, the parameter  $p_1$  in  $[q]_{q-p_1}^{[q]}$  represents the number of coalescences of the change of index mapping  $a$ . The  $p_2$  is the number of  $b(i)$  such that  $b(i) = 0$  or  $x_z^{(a,b),i} = z$ ; it will be referred to as the number of  $z$ -infections of the mapping  $b$ .

We recall that the Stirling numbers of the second kind  $S(q, p)$  is the number of partitions of  $[q]$  into  $p$  sets, so that

$$\# \left( [r]_p^{[q]} \right) = S(q, p) (r)_p \quad \text{and} \quad r^q = \sum_{1 \leq p \leq q} S(q, p) (r)_p$$

for any  $p \leq q \leq r$ . We also recall that the Stirling numbers of the first kind  $s(q, p)$  provide the coefficients of the polynomial expansion of  $(r)_q$

$$(r)_q = \sum_{1 \leq p \leq q} s(q, p) r^p \quad (4.1)$$

We also use the conventions  $(r)_q = 0$  and  $(r)_0 = 1 = (-r)_0$  for any  $q > r \geq 0$ , as well as  $s(q, 0) = s(0, -q) = S(0, -q) = S(q, 0) = 0$  except  $s(0, 0) = S(0, 0) = 1$ , for  $q = 0$ .

These formulae can be found in any textbook on combinatorial analysis, see for instance [11, 12].

**Definition 4.6** We also consider the sequence of probabilities  $\mathcal{P}^{(N,q)} = \mathcal{P}^{[N,q,1]} \otimes \mathcal{P}^{[N,q,2]}$  on the set  $\mathcal{I}_q$  defined by

$$\mathcal{P}^{(N,q)}(p_1, p_2) := \underbrace{\frac{1}{(N-1)^q} S(q, q-p_1) (N-1)_{q-p_1}}_{\mathcal{P}^{[N,q,1]}(p_1)} \times \underbrace{\binom{q}{p_2} \left(1 - \frac{1}{N}\right)^{q-p_2} \frac{1}{N^{p_2}}}_{\mathcal{P}^{[N,q,2]}(p_2)} \quad (4.2)$$

Notice that  $\mathcal{P}^{[N,q,1]}(p_1) = \# \left( [N-1]_{q-p_1}^{[q]} \right) / \# [N-1]^{[q]}$  is a statistics for the number of coalescences, whereas  $\mathcal{P}^{[N,q,2]}(p_2)$  is the proportion of infested mappings with  $p_2$  infections. By construction, we have the following lemma.

**Lemma 4.7** For any  $q < N$ , we have the formula

$$\mathbb{C}_z^{(N,q)} = \sum_{p \in \mathcal{I}_{0,q}} \mathcal{P}^{(N,q)}(p) \widehat{\mathbb{C}}_{z,p}^{(q)} \quad \text{with} \quad \widehat{\mathbb{C}}_{z,p}^{(q)} = \sum_{c \in \mathcal{I}_q(p)} \mathcal{C}_p^{(q)}(c) \mathbb{C}_{z,c}^{(q)}$$

We end this section with a Taylor expansion of the measure  $\mathcal{P}^{(N,q)}$  introduced above.

**Proposition 4.8** For any  $q < N$ , the mapping  $N \mapsto \mathcal{P}^{(N,q)}$  is differentiable at any order  $m \geq 0$ . The  $m$ -order derivative is supported by

$$\mathcal{T}_{q,n}^{(m)} := \{(p_1, p_2) \in \mathcal{I}_q : 0 \leq p_1 + p_2 \leq m\}.$$

Indeed, Fla (4.2) shows that the fraction in the variable  $N$ ,  $\mathcal{P}^{(N,q)}(p_1, p_2)$ , can be expanded as a formal power series in  $\frac{1}{N}$  (or, more precisely, as an analytic function in the neighborhood of 0) with leading term in  $\frac{1}{N^{p_1+p_2}}$ . The Proposition follows.

Expanding the formula for  $\mathcal{P}^{(N,q)}(p_1, p_2)$  using (4.1) and the Taylor expansion

$$\frac{1}{(1-x)^n} = \sum_{0 \leq k} (n+k-1)_k \frac{x^k}{k!} = \sum_{0 \leq k} \binom{n+k-1}{k} x^k$$

with  $(n-1)_0 := 1$ , we get an explicit formula for the derivatives.

**Proposition 4.9** *The  $m$ -th order derivative is given by the signed measure (with total null mass) supported on the set  $\mathcal{T}_{q,n}^{(m)}$ :*

$$d^{(m)}\mathcal{P}^{(q)} := \sum_{(p_1, p_2) \in \mathcal{T}_{q,n}^{(m)}} \tau_{q,p_1,p_2}^{(m)} \delta_{(p_1, p_2)}, \quad (4.3)$$

with

$$\tau_{q,p_1,p_2}^{(m)} = \sum_{\mathbf{k} \in \mathbb{K}_q^{(m)}(p_1, p_2)} \alpha_{q,p_1,p_2}(\mathbf{k}),$$

$$\mathbb{K}_q^{(m)}(p_1, p_2) := \left\{ (k_1, k_2, k_3) \in [0, q - p_1] \times [0, q - p_2] \times \mathbb{N} : \sum_{1 \leq i \leq 2} p_i + \sum_{1 \leq i \leq 3} k_i = m \right\},$$

$$\begin{aligned} \alpha_{q,p_1,p_2}(k_1, k_2, k_3) &= S(q, q - p_1) \binom{q}{p_2} \\ &\times s(q - p_1, q - p_1 - k_1) (-1)^{k_2} \binom{q - p_2}{k_2} \binom{(p_1 + k_1) + k_3 - 1}{k_3}. \end{aligned}$$

**Remark 4.10** *We observe that  $\tau_{q,p_1,p_2}^{(0)} = 1_{(0,0)}(p_1, p_2)$ . As will appear later on, this identity encodes the propagation of chaos properties (i.e. asymptotic independency) of PMCMC samplers. We also mention that  $\alpha_{q,p_1,p_2}(\mathbf{k}) = 0 = \tau_{q,p_1,p_2}^{(m)}$  as soon as  $p_1 > q$  or  $p_2 > q$ .*

**Remark 4.11** *The  $m$ -th order signed measure  $d^{(m)}\mathcal{P}^{(q)}$  and the mapping  $(p_1, p_2) \mapsto \tau_{q,p_1,p_2}^{(m)}$  in formula (4.3) only charge couple of integers  $(p_1, p_2) \in ([1, q] \times [0, q])$  s.t.  $0 \leq p_1 + p_2 \leq m$ . The first coordinate  $0 \leq p_1 < q$  can be interpreted as the number of coalescent states, while  $p_2$  can be interpreted as the the number of  $z$ -infected states.*

*By construction, the mapping  $(p_1, p_2) \mapsto \tau_{q,p_1,p_2}^{(m)}$  can also be seen as a measure with null total mass supported on the set  $0 \leq p_1 + p_2 \leq m$ . For instance, for  $m = 1, 2$ , recalling that  $s(q, q - 1) = -q(q - 1)/2 = -S(q, q - 1)$ ,  $s(q, q - 2) = \frac{q!}{3!(q-3)!} \frac{3q-1}{4}$ , and  $S(q, q - 2) = \frac{q!}{3!(q-3)!} (3q - 5)/4$ , we have*

$$\begin{aligned} \tau_{q,2,0}^{(2)} &= \frac{q!}{3!(q-3)!} \frac{3q-5}{4} & \tau_{q,0,2}^{(2)} &= \frac{q(q-1)}{2} \\ \tau_{q,0,0}^{(2)} &= \frac{q^2(q-1)}{2} + \frac{q!}{3!(q-3)!} \frac{3q-1}{4} & \tau_{q,1,0}^{(2)} &= -\left(\frac{q(q-1)}{2}\right)^2 \\ \tau_{q,0,1}^{(2)} &= -\frac{q^2(q-1)}{2} - q(q-1) & \tau_{q,1,1}^{(2)} &= q \frac{q(q-1)}{2} \\ \tau_{q,1,0}^{(1)} &= \frac{q(q-1)}{2} & \tau_{q,0,1}^{(1)} &= q & \tau_{q,0,0}^{(1)} &= -(\tau_{q,1,0}^{(1)} + \tau_{q,0,1}^{(1)}) \end{aligned} \quad (4.4)$$

**Definition 4.12** *We denote by  $\mathbf{p}_n := (p_0, \dots, p_n)$  a given multi-index in  $\mathcal{I}_{n,q} := (\mathcal{I}_q)^{n+1}$ , with  $p_k = (p_k^1, p_k^2) \in \mathcal{I}_q$  for any  $0 \leq k \leq n$ . We also denote by  $\mathbf{c}_n = (c_0, \dots, c_n)$  a sequence of mappings in the set*

$$\mathcal{J}_{q,n} = \cup_{\mathbf{p}_n \in \mathcal{I}_{n,q}} \mathcal{I}_q(\mathbf{p}_n) \quad \text{with} \quad \mathcal{I}_q(\mathbf{p}_n) := \prod_{0 \leq k \leq n} \mathcal{I}_q(p_k)$$

*For any  $\mathbf{m}_n = (m_0, \dots, m_n) \in \mathbb{N}^{n+1}$ , we set  $|\mathbf{m}_n| = \sum_{0 \leq k \leq n} m_k$ , and we use the multi-index notation*

$$\tau_{q,\mathbf{p}_n}^{(\mathbf{m}_n)} = \prod_{0 \leq k \leq n} \tau_{q,p_k^1,p_k^2}^{(m_k)}, \quad \tau_{q,\mathbf{p}_n}^{(m)} := \sum_{|\mathbf{m}_n|=m} \tau_{q,\mathbf{p}_n}^{(\mathbf{m}_n)}, \quad \mathcal{T}_{q,n}^{(m)} := \prod_{|\mathbf{m}_n|=m} \prod_{0 \leq k \leq n} \mathcal{T}_{q,n}^{(m_k)}$$

and

$$\mathcal{C}_{\mathbf{p}_n}^{(q)}(\mathbf{c}_n) := \prod_{0 \leq k \leq n} \mathcal{C}_{p_k}^{(q)}(c_k) \quad \mathcal{P}_n^{(N,q)}(\mathbf{p}_n) := \prod_{0 \leq k \leq n} \mathcal{P}^{(N,q)}(p_k)$$

In this notation, and recalling that  $p_n^1 + p_n^2 > m_n \Rightarrow \tau_{q, p_n}^{(m_n)} = 0$ , we readily prove the following extension of lemma 4.9

**Proposition 4.13** *For any  $q < N$  and  $n \geq 0$ , the mapping  $N \mapsto \mathcal{P}_n^{(N, q)}$  is differentiable at any order. In addition, the  $m$ -th order derivative is the signed measure with null mass*

$$d^{(m)} \mathcal{P}_n^{(q)} = \sum_{p_n \in \mathcal{T}_{q, n}^{(m)}} \tau_{q, p_n}^{(m)} \delta_{p_n}$$

**Definition 4.14** *For further use, let  $\mathbf{c} = (c_0, \dots, c_n)$ ,  $c_i = (a_i, b_i)$  be a sequence of mappings in the set  $\mathcal{J}_{q, n}$ , and let us say that*

- the  $p$ -th trajectory,  $1 \leq p \leq q$  of  $\mathbf{c}$  is free if  $\forall i \leq n, \forall m \neq p$ ,

$$a_i \circ \dots \circ a_n(p) \neq a_i \circ \dots \circ a_n(m) \text{ and } b_i(a_{i+1} \circ \dots \circ a_n(p)) \neq 1$$

- the  $p$ -th trajectory is coalescent if  $\exists i \leq n, \exists m \neq p, a_i \circ \dots \circ a_n(p) = a_i \circ \dots \circ a_n(m)$
- the  $p$ -th trajectory is infected if  $\exists i \leq n, b_i(a_{i+1} \circ \dots \circ a_n(p)) = 1$ .

## 4.2 Unnormalized tensor product measures

Let us apply now these combinatorial results to PMCMC samplers. Our first result is concerned with tensor product measures. Given a frozen trajectory  $z := (z_n)_{n \geq 0} \in \prod_{n \geq 0} S_n$ , we denote by  $\mathcal{X}_{z, n}$  the dual mean field model associated with the Feynman-Kac particle model  $\mathcal{X}_n$  and the frozen path  $X_n = z_n$ .

We also set

$$\eta_{z, n}^N := m(\mathcal{X}_{z, n}) = m_{z_n}(\mathcal{X}_{z, n}^-), \quad \gamma_{z, n}^N(1) := \prod_{0 \leq p < n} \eta_{z, p}^N(G_p), \quad \gamma_{z, n}^N := \gamma_{z, n}^N(1) \cdot \eta_{z, n}^N,$$

and finally, for any function  $F$  on  $S_n^q$

$$\Upsilon_{z, n}^{(N, q)}(F) := \mathbb{E}((\gamma_{z, n}^N)^{\otimes q}(F)) / \gamma_n(1)^q.$$

**Definition 4.15** *We consider the tensor product measures*

$$\Delta_{z, p_n}^{(q)} = \left( \eta_0^{\otimes q} \widehat{\mathbb{C}}_{z_0, p_0}^{(q)} \right) \left( \overline{Q}_1^{\otimes q} \widehat{\mathbb{C}}_{z_1, p_1}^{(q)} \right) \dots \left( \overline{Q}_n^{\otimes q} \widehat{\mathbb{C}}_{z_n, p_n}^{(q)} \right) = \sum_{\mathbf{c}_n \in \mathcal{I}_q(p_n)} \mathcal{C}_{p_n}^{(q)}(\mathbf{c}_n) \Delta_{z, \mathbf{c}_n}^{(q)} \quad (4.5)$$

with the conditional expectation operators

$$\Delta_{z, \mathbf{c}_n}^{(q)} := \left( \eta_0^{\otimes q} \mathbb{C}_{z_0, c_0}^{(q)} \right) \left( \overline{Q}_1^{\otimes q} \mathbb{C}_{z_1, c_1}^{(q)} \right) \dots \left( \overline{Q}_n^{\otimes q} \mathbb{C}_{z_n, c_n}^{(q)} \right)$$

**Theorem 4.16** *For any  $q < N$ ,  $n \geq 0$ , we have*

$$\Upsilon_{z, n}^{(N, q)} = \sum_{p_n \in \mathcal{I}_{n, q}} \sum_{\mathbf{c}_n \in \mathcal{I}_q(p_n)} \left[ \mathcal{P}_n^{(N, q)}(p_n) \mathcal{C}_{p_n}^{(q)}(\mathbf{c}_n) \right] \Delta_{z, \mathbf{c}_n}^{(q)}$$

**Proof:**

By construction, we have  $\eta_{z, n}^N := m_{z_n}(\mathcal{X}_{z, n}^-)$  and

$$m_{z_n}(\mathcal{X}_{z, n}^-)^{\otimes q} = m(\mathcal{X}_{z, n}^-)^{\otimes q} \mathbb{C}_{z_n}^{(N, q)}$$

On the other hand, for any function  $F$  on  $S_n^q$  we have

$$\mathbb{E} \left( m(\mathcal{X}_{z,n+1}^-)^{\odot q}(F) \mid \mathcal{F}_n \right) = (\eta_{z,n}^N)^{\otimes q} \left( Q_{n+1}^{\otimes q}(F) \right) / \eta_{z,n}^N(G_n)^q$$

This implies that

$$\begin{aligned} \mathbb{E} \left( (\gamma_{z,n+1}^N)^{\otimes q}(F) \mid \mathcal{F}_n \right) &= \gamma_{z,n}^N(1)^q \times (\eta_{z,n}^N)^{\otimes q} \left( Q_{n+1}^{\otimes q} \mathbb{C}_{z_{n+1}}^{(N,q)}(F) \right) \\ &= (\gamma_{z,n}^N)^{\otimes q} \left( Q_{n+1}^{\otimes q} \mathbb{C}_{z_{n+1}}^{(N,q)}(F) \right) \end{aligned}$$

from which we conclude that

$$\Upsilon_{z,n}^{(N,q)}(F) = \left( \eta_0^{\otimes q} \mathbb{C}_{z_0}^{(N,q)} \right) \left( \overline{Q}_1^{\otimes q} \mathbb{C}_{z_1}^{(N,q)} \right) \dots \left( \overline{Q}_n^{\otimes q} \mathbb{C}_{z_n}^{(N,q)} \right) (F).$$

The Theorem follows by expanding the  $\mathbb{C}_{z_i}^{(N,q)}$  in terms of the  $\mathbb{C}_{z_i, c_i}^{(q)}$ . ■

The next corollary is a direct consequence of the proof of theorem 4.16. It provides a more probabilistic description of the measure  $\Upsilon_n^{(N,q)}$  in terms of expectation operators.

**Corollary 4.17** *For any  $q < N$ ,  $n \geq 0$ ,  $\Upsilon_{z,n}^{(N,q)}$  is differentiable at any order. In addition, its derivatives are for any  $n \geq 0$  given by the recursion*

$$d^{(m)} \Upsilon_{z,n}^{(q)}(F) = \sum_{r_1+r_2=m} \sum_{p \in \mathcal{I}_q} d^{(r_1)} \mathcal{P}^{(q)}(p) d^{(r_2)} \Upsilon_{z,n-1}^{(q)} \left( \overline{Q}_n^{\otimes q} \widehat{\mathbb{C}}_{z_n,p}^{(q)}(F) \right)$$

with the conventions  $\Upsilon_{z,-1}^{(q)} \overline{Q}_0^{\otimes q} = \eta_0^{\otimes q}$  and  $d^{(r_2)} \Upsilon_{z,-1}^{(q)} \overline{Q}_0^{\otimes q} = 0$  for  $r_2 > 0$ . In particular we get the expansions

$$d^{(m)} \Upsilon_{z,n}^{(q)} = \sum_{\mathbf{p}_n \in \mathcal{T}_{q,n}^{(m)}} \tau_{\mathbf{q}, \mathbf{p}_n}^{(m)} \times \Delta_{z, \mathbf{p}_n}^{(q)}. \quad (4.6)$$

For further use, let us study further the action of the operators  $\Delta_{z, \mathbf{c}_n}^{(q)}$ . We already know that they contribute to  $d^{(m)} \Upsilon_{z,n}^{(q)}$  only if the total number of coalescences and infections of  $\mathbf{c}_n$ , written  $Tot(\mathbf{c}_n)$  is less than  $m$ .

**Lemma 4.18** *Let  $f$  a  $\eta_n$ -centered function on  $S_n$  ( $\eta_n(f) = 0$ ). Then, for any sequence of mappings  $\mathbf{c}_n$ ,*

$$Tot(\mathbf{c}_n) < \frac{q}{2} \Rightarrow \Delta_{z, \mathbf{c}_n}^{(q)}(f^{\otimes q}) = 0.$$

*In particular,  $d^{(m)} \Upsilon_{z,n}^{(q)}(f^{\otimes q}) = 0$  whenever  $m < \frac{q}{2}$ .*

Indeed, let us assume that  $Tot(\mathbf{c}_n) < \frac{q}{2}$ . It follows immediately that one trajectory is free in the sense of Definition 4.14. Because of the symmetry of the problem (which, as usual, is invariant by permutation of the particles), we may assume without restriction that the particles of this free trajectory all have the same index  $q$  ( $a_i(q) = q \forall i \leq n$ ). Let us write  $\hat{\mathbf{c}}_n$  for the sequence of mappings obtained by restricting each  $a_i$  to a map from  $[q-1]$  to itself (this process is well-defined because of the freeness assumption) and by restricting similarly  $b_i$  to  $[q-1]$ . It follows then from the very definition of  $\Delta_{z, \mathbf{c}_n}^{(q)}(f^{\otimes n})$  that

$$\Delta_{z, \mathbf{c}_n}^{(q)}(f^{\otimes q}) = \Delta_{z, \hat{\mathbf{c}}_n}^{(q-1)}(f^{\otimes q-1}) \cdot \eta_n(f) = 0.$$

The Lemma follows.



**Corollary 4.19** *We have for an arbitrary  $q \leq N$ :*

$$\mathbb{E}[(\gamma_{z,n}^N(G_n - \eta_n(G_n)))^q] = \mathbb{E}[(\gamma_{z,n}^N)^{\otimes q}((G_n - \eta_n(G_n))^{\otimes q})] = O(N^{-q/2}).$$

**Corollary 4.20** *We have for an arbitrary  $q \leq N$ :*

$$\mathbb{E}[(\gamma_{z,n}^N(G_n) - \gamma_n(G_n))^q] = O(N^{-q/2}).$$

Indeed,

$$\begin{aligned} \gamma_{z,n}^N(G_n) - \gamma_n(G_n) &= \prod_{0 \leq p \leq n} \eta_{z,n}^N(G_n) - \prod_{0 \leq p \leq n} \eta_n(G_n) \\ &= \gamma_{z,n}^N(G_n - \eta_n(G_n)) + [\gamma_{z,n-1}^N(G_{n-1}) - \gamma_{n-1}(G_{n-1})]\eta_n(G_n) \\ &= \sum_{i=0}^n [\gamma_{z,i}^N(G_i - \eta_i(G_i))] \prod_{j=i+1}^n \eta_j(G_j). \end{aligned}$$

The proof follows from the previous Corollary and the Minkowski identity.

### 4.3 Normalized tensor product measures

In the present paragraph, we show that the distribution  $\mathbb{P}_{z,n+1}^{(N,q)}$  of the first  $q$  random non frozen particles (see definition 3.18) has derivatives at all orders.

We recall the instrumental identity: for any  $u \neq 1$ ,  $q \geq 0$  and  $m \geq 1$

$$\frac{1}{(1-u)^{q+1}} = \sum_{0 \leq k \leq m} (q+k)_k \frac{u^k}{k!} + u^m \sum_{1 \leq k \leq q+1} \binom{(q+1)+m}{k+m} \left(\frac{u}{1-u}\right)^k \quad (4.7)$$

A detailed proof of this result can be found in [22] (cf. lemma 4.11 on page 820).

Using the identity  $\binom{n+1}{k} = \sum_{k \leq l \leq n} \binom{n}{l}$  (following e.g. from  $1 - (1-x)^{n+1} = x \sum_{0 \leq k \leq n} (1-x)^k$ ), we get

$$\frac{1}{x^q} = \frac{(q+r)!}{(q-1)!} \sum_{0 \leq l \leq r} \frac{1}{(q+l)} \frac{(-1)^l}{l!(r-l)!} x^l + O((1-x)^{r+1}) \quad (4.8)$$

**Theorem 4.21** *For any  $q < N$ ,  $n \geq 0$ , and any  $r \geq 1$  we have*

$$\mathbb{P}_{z,n+1}^{(N,q)} = \eta_{n+1}^{\otimes q} + \sum_{1 \leq k \leq \lfloor (N-q)/2 \rfloor} \frac{1}{N^k} d^{(k)} \mathbb{P}_{z,n+1}^{(q)} + O\left(\frac{1}{N^{((N-q)+1)/2}}\right)$$

with the  $k$ -th order derivatives given for any function  $F$  on  $S_n^q$  by

$$d^{(k)} \mathbb{P}_{z,n+1}^{(q)}(F) = \frac{(q+2k)!}{(q-1)!} \sum_{0 \leq l \leq 2k} \frac{(-1)^l}{(q+l)} \frac{1}{l!(2k-l)!} d^{(k)} \Upsilon_{z,n}^{(l+q)} \left[ \overline{Q}_{n,n+1}^{\otimes(l+q)}(1^{\otimes l} \otimes F) \right] \quad (4.9)$$

Following the proof of theorem 4.16 we find that

$$\mathbb{E} \left( m(\mathcal{X}_{z,n+1}^-)^{\odot q}(F) \right) = \mathbb{E} \left[ \gamma_{z,n}^N(\overline{G}_n)^{-q} \times (\gamma_{z,n}^N)^{\otimes q} \left( \overline{Q}_{n,n+1}^{\otimes q}(F) \right) \right]$$

Combining (4.8) with Corollary 4.20 we find that

$$\begin{aligned} &\mathbb{E} \left( m(\mathcal{X}_{z,n+1}^-)^{\odot q}(F) \right) + O\left(\frac{1}{N^{(r+1)/2}}\right) \\ &= \frac{(q+r)!}{(q-1)!} \sum_{0 \leq l \leq r} \frac{1}{(q+l)} \frac{(-1)^l}{l!(r-l)!} \mathbb{E} \left( (\gamma_{z,n}^N)^{\otimes(l+q)} \left( \overline{G}_n^{\otimes l} \otimes (\overline{Q}_{n,n+1}^{\otimes q}(F)) \right) \right) \end{aligned}$$

for any  $r \geq 0$ . We prove then (4.9) using the fact that

$$\overline{G}_n^{\otimes l} \otimes \left( \overline{Q}_{n,n+1}^{\otimes q}(F) \right) = \overline{Q}_{n,n+1}^{\otimes(q+l)}(1^{\otimes l} \otimes F)$$

and choosing  $r = 2k$ , with  $0 \leq k \leq \lfloor (N - q)/2 \rfloor$ . This ends the proof of the theorem.  $\blacksquare$

It is instructive to derive explicit expressions for the derivatives –this will be one of the topics addressed in the forthcoming paragraphs. Let us anticipate on these developments and make explicit the first order derivative in a simple case. For  $k = q = 1$ , and any function  $f$  on  $S_n$ , with  $\eta_n(f) = 0$ , using the first order expansions that will be stated in corollary 4.24 it is readily checked that

$$d^{(1)}\mathbb{P}_{z,n+1}^{(1)}(f) = \sum_{0 \leq k \leq n} \overline{Q}_{k,n+1}(f)(z_k) - \sum_{0 \leq k \leq n} \eta_k(\overline{Q}_{k,n+1}(1)\overline{Q}_{k,n+1}(f)).$$

## 4.4 Infected forest expansions

We know that  $\mathbb{P}_{z,n}^{(q,N)}$  has derivatives at all orders and can be expanded in terms of the derivatives of  $\Upsilon_{z,n}^{(N)}$ . In turn, these last derivatives can be expanded in terms of the elementary integral operators  $\Delta_{z,n,c}^{(q)}$ . However, because of the symmetries of Feynman-Kac models, many of these operators coincide and this expansion is not efficient, neither computationally nor theoretically. The present paragraph aims at clarifying these questions and get rid of redundancies in combinatorial expansions of derivatives.

The results in this paragraph build largely on [22]. We will therefore skip the details of the arguments that follow closely the ones in [22] and refer simply the reader to that article for further details on the definitions, proofs, reasonings and so on on trees, forests and jungles.

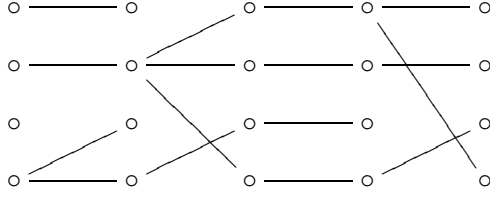
### 4.4.1 Forests and jungles

We start with recalling some more or less classical terminology on trees and forests introduced in [22].

A tree is a (isomorphism class of) finite non-empty oriented connected graph  $\mathbf{t}$  without loops such that any vertex of  $\mathbf{t}$  has at most one outgoing edge. Paths are oriented from the vertices to the root. The height of a tree is the maximum length of a path. Similarly, the level of a vertex in a tree is the length of the path that connects it to the root. These definition will extend in a straightforward way to the objects to be introduced below (forests and jungles).

A forest  $\mathbf{f}$  is a multi-set of trees, that is a set of trees, with repetitions of the same tree allowed, or equivalently an element of the commutative monoid  $\langle \mathcal{T} \rangle$  on  $\mathcal{T}$ , with the empty graph  $T_0 = \emptyset$  as a unit. Since the algebraic notation is the most convenient, we write  $\mathbf{f} = \mathbf{t}_1^{m_1} \dots \mathbf{t}_k^{m_k}$ , for the forest with the tree  $\mathbf{t}_i$  appearing with multiplicity  $m_i$ ,  $i \leq k$ . When  $\mathbf{t}_i \neq \mathbf{t}_j$  for  $i \neq j$ , we say that  $\mathbf{f}$  is written in normal form. The sets of forests with height  $(n + 1)$ , and with  $q$  vertices at each level set is written  $Forest_{q,n}$ .

To a sequence  $\mathbf{a} = (a_0, \dots, a_n) \in \mathcal{A}_{q,n} := ([q]^{[q]})^{n+1}$  is naturally associated a forest  $F(\mathbf{a})$ : the one with one vertex for each element of  $[q]^{n+1}$ , and a edge for each pair  $(i, a_k(i)), i \in [q]$ . The sequence can also be represented graphically uniquely by a planar graph  $J(\mathbf{a})$ , where however the edges between vertices at level  $k + 1$  and  $k$  are allowed to cross. We call such a planar graph, where paths between vertices are entangled, a *jungle*. The set of such jungles is written  $Jungle_{q,n}$ . Here is the graphical representation of a jungle (for consistency with the probabilistic interpretation of heights and levels as time-indices, we represent trees, forest and jungles *horizontally* and from left to right –roots are on the left !).



The group  $\mathcal{G}_{q,n} := \mathcal{G}_q^{n+2}$  also acts naturally on sequences of maps  $\mathbf{a} \in \mathcal{A}_{q,n}$ , and on jungles  $J(\mathbf{a}) \in \text{Jungle}_{q,n}$  by permutation of the vertices at each level. More precisely, for all  $\mathbf{a} \in \mathcal{A}_{n,q}$  and all  $\sigma = (\sigma_0, \dots, \sigma_{n+1}) \in \mathcal{G}_{q,n}$  by the pair of formulae

$$\sigma(\mathbf{a}) := (\sigma_0 a_0 \sigma_1^{-1}, \sigma_1 a_1 \sigma_2^{-1}, \dots, \sigma_n a_n \sigma_{n+1}^{-1}) \quad \text{and} \quad \sigma J(\mathbf{a}) := J(\sigma(\mathbf{a})) \quad (4.10)$$

Notice that if two sequences  $\mathbf{a}$  and  $\mathbf{a}' \in \mathcal{A}_{q,n}$  differ only by the order of the vertices in  $J(\mathbf{a})$  and  $J(\mathbf{a}')$  (i.e. by the action of an element of  $\mathcal{G}_{q,n}$ ) then the associated forests are identical:  $F(\mathbf{a}) = F(\mathbf{a}')$ . The converse is also true: if  $F(\mathbf{a}) = F(\mathbf{a}')$ , then  $J(\mathbf{a})$  and  $J(\mathbf{a}')$  differ only by the ordering of the vertices, since they have the same underlying non planar graph. In this situation,  $\mathbf{a}$  and  $\mathbf{a}'$  belong to the same orbit

$$[\mathbf{a}] := \{\sigma(\mathbf{a}) : \sigma \in \mathcal{G}_{q,n}\}$$

under the action of  $\mathcal{G}_{q,n}$ . In particular, the set of equivalence classes of jungles in  $\text{Jungle}_{q,n}$  under the action of the permutation groups  $\mathcal{G}_{q,n}$  is in bijection with both the set of  $\mathcal{G}_{q,n}$ -orbits of maps in  $\mathcal{A}_{q,n}$  and the set of forests  $\text{Forest}_{q,n}$ . Writing  $\text{Stab}(\mathbf{a}) := \{\tau \in \mathcal{G}_{q,n} : \tau(\mathbf{a}) = \mathbf{a}\}$  for the stabilizer subgroup of  $\mathbf{a}$ , the class formula yields

$$\#[\mathbf{a}] = \#\mathcal{G}_{q,n} / \#\text{Stab}(\mathbf{a}) = (q!)^{n+2} / \#\text{Stab}(\mathbf{a}).$$

To compute the cardinality of the set  $\text{Stab}(\mathbf{a})$  in terms of forests and trees, we denote by  $\text{Cut}(\mathbf{t})$  the forest deduced from cutting the root of the tree  $\mathbf{t}$ ; that is, removing its root vertex, and all its incoming edges. In the reverse angle, we denote by  $\text{Cut}^{-1}(\mathbf{f})$  the tree deduced from the forest  $\mathbf{f}$  by adding a common root to its rooted tree. The symmetry multiset  $\mathbf{S}(\mathbf{t})$  of a tree  $\mathbf{t} = \text{Cut}^{-1}(\mathbf{t}_1^{m_1} \dots \mathbf{t}_k^{m_k})$  associated with a forest written in normal form, is defined by  $\mathbf{S}(\mathbf{t}) := (m_1, \dots, m_k)$ . The symmetry multiset of a forest is given by

$$\mathbf{S}(\mathbf{t}_1^{m_1} \dots \mathbf{t}_k^{m_k}) := \left( \underbrace{\mathbf{S}(\mathbf{t}_1), \dots, \mathbf{S}(\mathbf{t}_1)}_{m_1\text{-terms}}, \dots, \underbrace{\mathbf{S}(\mathbf{t}_k), \dots, \mathbf{S}(\mathbf{t}_k)}_{m_k\text{-terms}} \right)$$

We also extend  $\text{Cut}(\mathbf{f})$  to forests  $\mathbf{f} = \mathbf{t}_1^{m_1} \dots \mathbf{t}_k^{m_k}$  by setting

$$\text{Cut}(\mathbf{f}) = \text{Cut}(\mathbf{t}_1)^{m_1} \dots \text{Cut}(\mathbf{t}_k)^{m_k} \quad (4.11)$$

where  $\text{Cut}(\mathbf{t}_i)^{m_i}$  stands for the forest deduced from  $\text{Cut}(\mathbf{t}_i)$  repeated  $m_i$  times. Combining the class formula with a recursion with respect to the height parameter, we obtain

$$\#[[\mathbf{a}]] = (q!)^{n+2} / \#(\text{Stab}(\mathbf{a})) \quad \text{with} \quad \#(\text{Stab}(\mathbf{a})) = \prod_{i=-1}^n \mathbf{S}(\text{Cut}^i(F(\mathbf{a})))! \quad (4.12)$$

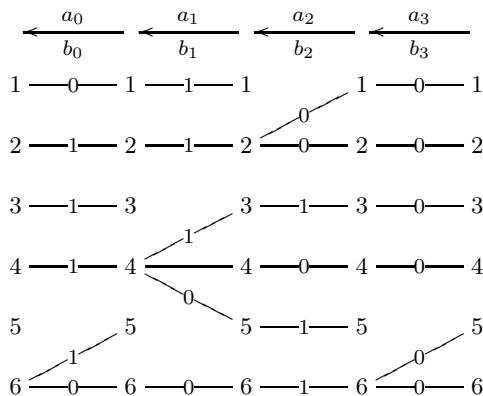
where we have used the multi-index factorial notation  $(n_1, \dots, n_k) = n_1! \dots n_k!$ , for any  $n_k \in \mathbb{N}$ , with  $k \geq 0$ . A detailed proof of this closed formula is provided in [22].

We let the reader check that, for example, for  $\mathbf{a}$  as in the above graphical representation,  $\#(\text{Stab}(\mathbf{a})) = 1 \cdot 1 \cdot 2! \cdot 2! = 4$  and  $\#[[\mathbf{a}]] = (4!)^4 \cdot 3!$ .

### 4.4.2 Infected forests

Recall that the study of PMCMC samplers requires the introduction of sequences of mappings  $\mathbf{c} = (\mathbf{a}, \mathbf{b}) \in \mathcal{J}_{q,n}$ , where the maps  $b_k$  can be thought of as “infections” (using the terminology previously introduced). The infection of a jungle  $J(\mathbf{a})$  (or of the associated sequence of maps  $\mathbf{a}$ ) is defined accordingly by a sequence of functions  $\mathbf{b} = (b_0, \dots, b_n) \in (\{0, 1\}^{[q]})^{n+1}$ .

Graphically, the infection is represented by the label 1, and the non infection by the label 0 on the edges of the jungle. The diagram below provides an example of infected planar forest of height 4 with 5 trees and 6 leaves, and the corresponding sequence of infection mappings.



By construction, there are  $\prod_{0 \leq k \leq n} \binom{q}{i_k}$  ways of infecting a given forest with  $0 \leq i_k \leq q$  infections at each level  $0 \leq k \leq n$ . Some of them are clearly equivalent. To be more precise, we consider the following equivalence relation on infected jungles

$$(\mathbf{a}, \mathbf{b}) \sim (\mathbf{a}', \mathbf{b}') \iff \exists \sigma \in \mathcal{G}_{q,n} : \sigma(\mathbf{a}, \mathbf{b}) = (\mathbf{a}', \mathbf{b}')$$

The equivalence classes are denoted by

$$[\mathbf{a}, \mathbf{b}] := \{ \sigma(\mathbf{a}, \mathbf{b}) : \sigma \in \mathcal{G}_{q,n} \} = \{ (\sigma(\mathbf{a}), \mathbf{b}\bar{\sigma}^{-1}) : \sigma \in \mathcal{G}_{q,n} \}$$

with

$$\bar{\sigma} := (\sigma_1, \dots, \sigma_{n+1}) \quad \text{and} \quad \bar{\sigma}^{-1} = (\sigma_1^{-1}, \dots, \sigma_{n+1}^{-1})$$

The definitions of forests and jungles discussed in the previous section extend also in a straightforward way to the infected case (edges being colored by 0 or 1). To a sequence  $(\mathbf{a}, \mathbf{b})$  is then naturally associated an infected forest  $F(\mathbf{a}, \mathbf{b})$ : the one with one vertex for each element of  $[q]^{n+1}$ , and an infected edge for each triplet  $(i, b_k(i), a_k(i)), i \in [q]$ . The set of infected forests is in bijection with the set of  $\mathcal{G}_{q,n}$ -orbits of maps in  $\mathcal{J}_{q,n}$ .

The class formula yields once again a way to compute the cardinals of the classes  $[\mathbf{a}, \mathbf{b}]$  from the action of the symmetry group  $\mathcal{G}_{q,n}$ .

**Lemma 4.22** *The number of infected jungles in  $[\mathbf{a}, \mathbf{b}]$  is given by*

$$\#[\mathbf{a}, \mathbf{b}] = (q!)^{n+2} / \text{Stab}_{\mathbf{a}}(\mathbf{b}) = \#[\mathbf{a}] \times \frac{\#(\text{Stab}(\mathbf{a}))}{\#(\text{Stab}_{\mathbf{a}}(\mathbf{b}))}$$

with

$$\text{Stab}_{\mathbf{a}}(\mathbf{b}) := \{ \tau \in \text{Stab}(\mathbf{a}) : \mathbf{b}\bar{\tau} = \mathbf{b} \}.$$

As for the non infected case,  $\#(\text{Stab}_{\mathbf{a}}(\mathbf{b}))$  can be computed inductively, following essentially the same principles. We describe briefly how this can be done.

Let  $\mathbf{t}_1, \dots, \mathbf{t}_n$  and  $\mathbf{t}'_1, \dots, \mathbf{t}'_m$  be two families of distinct infected trees and  $l_i, i = 1 \dots n, p_j, j = 1 \dots m$  two sequences of positive integers. We write  $\mathbf{t}_1^{l_1} \dots \mathbf{t}_n^{l_n} \otimes \mathbf{t}'_1^{p_1} \dots \mathbf{t}'_m^{p_m}$  for the infected tree obtained by joining, for  $i = 1 \dots n$ ,  $l_i$  copies of  $\mathbf{t}_i$  to a common root with infection index 0 and for  $i = 1 \dots m$ ,  $p_i$  copies of  $\mathbf{t}'_i$  to the same common root with infection index 1. Any infected tree  $\mathbf{t}$  can be written uniquely in that way: we write  $\mathbf{S}'(\mathbf{t}) = (l_1, \dots, l_n, p_1, \dots, p_m)$  for the corresponding multiset and call it the symmetry multiset of  $\mathbf{t}$ .

Cuts of infected trees and infected forests are infected forests that are defined as in the non infected case by removing the root and erasing all infected edges connected to the root. A (right only) inverse operation  $\text{Cut}^{-1}$  acting on an infected forest  $\mathbf{t}_1^{k_1} \dots \mathbf{t}_n^{k_n}$  is defined by linking all the infected trees to a common root with non infected edges.

Mimicking the inductive arguments for counting jungles using cardinals of stabilizers in [22], we get

$$\text{Stab}_{\mathbf{a}}(\mathbf{b}) = \prod_{i=-1}^n \mathbf{S}'(\text{Cut}^i([\mathbf{a}, \mathbf{b}]))! \quad (4.13)$$

#### 4.4.3 Expectation operators on infected forests

Recall that  $\mathcal{J}_{q,n}$  is the set of  $(n+1)$  mappings  $\mathbf{c} = (\mathbf{a}, \mathbf{b}) = (c_0, \dots, c_n)$  with  $c_k = (a_k, b_k) \in I_q(p_k^1, p_k^2)$ , for any  $0 \leq k \leq n$ .

For any symmetric function  $F$  on  $S_n^q$ , and any  $\mathbf{c} = (\mathbf{a}, \mathbf{b})$  and  $\mathbf{c}' := (\mathbf{a}', \mathbf{b}')$  we have

$$\mathbf{c} \sim \mathbf{c}' \implies \Delta_{z,\mathbf{c}}^{(q)}(F) = \Delta_{z,\mathbf{c}'}^{(q)}(F)$$

We check this claim using the fact that for any  $a_1, a_2 \in [q]^{[q]}$ , and any  $b \in \{0, 1\}^{[q]}$ , and  $\sigma \in \mathcal{G}_q$  we have

$$\mathbb{A}_{a_1} \mathbb{A}_{a_2} = \mathbb{A}_{a_1 a_2} \quad \text{and} \quad \mathbb{B}_{z,b} = \mathbb{A}_{\sigma} \mathbb{B}_{z,b\sigma} \mathbb{A}_{\sigma^{-1}}$$

Thus, for any  $\mathbf{f} \in \mathcal{F}_{q,n}$  we can define unambiguously  $\Delta_{z,\mathbf{f}}^{(q)} = \Delta_{z,\mathbf{c}}^{(q)}$  for any choice  $\mathbf{c}$  of a representative of  $\mathbf{f}$  in  $\mathcal{J}_{q,n}$ .

We also denote by  $\mathcal{F}_q(\mathbf{p}_n)$  the set of forests with  $p_k^1$ -coalescences and  $p_k^2$  infections at each level  $0 \leq k \leq n$ . By construction, these forests are associated with the mappings  $\mathbf{c}_n \in \mathbf{I}_q(\mathbf{p}_n)$ . In this notation, the operators (4.5) can be rewritten in terms of the expectations operators on the set of infected forests

$$\Delta_{z,\mathbf{p}_n}^{(q)} = \sum_{\mathbf{c}_n \in \mathbf{I}_q(\mathbf{p}_n)} \mathbf{c}_{(\mathbf{p}_n)}^{(q)}(\mathbf{c}_n) \Delta_{z,\mathbf{c}_n}^{(q)} = \sum_{\mathbf{f} \in \mathcal{F}_q(\mathbf{p}_n)} \lambda_{q,\mathbf{p}_n}(\mathbf{f}) \Delta_{z,\mathbf{f}}^{(q)} \quad (4.14)$$

with the probability measure  $\lambda_{q,\mathbf{p}_n}$  given by

$$\lambda_{q,\mathbf{p}_n}(\mathbf{f}) = \#(\mathbf{f}) / \#(\mathbf{I}_q(\mathbf{p}_n)),$$

where we used the shortcut notation  $\#(\mathbf{f}) := \#[\mathbf{c}]$  for an arbitrary representative of  $\mathbf{f}$  in  $\mathcal{J}_{q,n}$ . We summarize the above discussion with the following theorem.

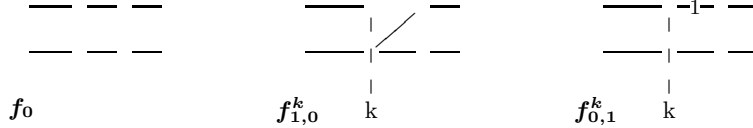
**Theorem 4.23** *For any  $m \geq 0$  we have*

$$d^{(m)} \Upsilon_{z,n}^{(q)} = \sum_{\mathbf{p}_n \in \mathcal{T}_{q,n}^{(m)}} \tau_{q,\mathbf{p}_n}^{(m)} \left( \sum_{\mathbf{f} \in \mathcal{F}_q(\mathbf{p}_n)} \lambda_{q,\mathbf{p}_n}(\mathbf{f}) \Delta_{z,\mathbf{f}}^{(q)} \right).$$

#### 4.4.4 Infected forests

The first order derivative is expressed in terms of two classes of infected forests. The explicit description of the second derivative depends on 20 different types of infected forests. We investigate them in this paragraph.

Let us fix  $3 < q < N$  and the time horizon  $n$ . There exists a single forest  $\mathbf{f}_0$  with trivial trees with no infection. There is also a single non infected forest  $\mathbf{f}_{1,0}^k$  with only one coalescence at level  $k$ . We also have a single forest  $\mathbf{f}_{0,1}^k$  with trivial trees and an infection at level  $k$ . A synthetic description of these forests is given below.



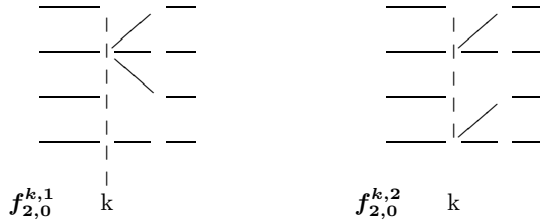
The corresponding measures are given by  $\Delta_{z,\mathbf{f}_0}^{(q)} = \eta_n^{\otimes q}$ , and the pair of measures

$$\Delta_{z,\mathbf{f}_{1,0}^k}^{(q)} = \eta_n^{\otimes(q-2)} \otimes \left[ \int \eta_k(dw) (\delta_w \overline{Q}_{k,n})^{\otimes 2} \right] \quad \text{and} \quad \Delta_{z,\mathbf{f}_{0,1}^k}^{(q)} = \eta_n^{\otimes(q-1)} \otimes \delta_{z_k} \overline{Q}_{k,n} \quad (4.15)$$

It is also immediate to check using (4.13) that

$$\#(\mathbf{f}_0) = q^{n+1} \quad \#(\mathbf{f}_{1,0}^k) = q^{n+2}/((q-2)!2!) \quad \text{and} \quad \#(\mathbf{f}_{0,1}^k) = q^{n+1} q$$

There are two non infected forests  $\mathbf{f}_{2,0}^{k,1}$  and  $\mathbf{f}_{2,0}^{k,2}$  with two coalescences at level  $k$ . The first one has a non trivial tree with three leaves, the second one has two trees with two leaves.



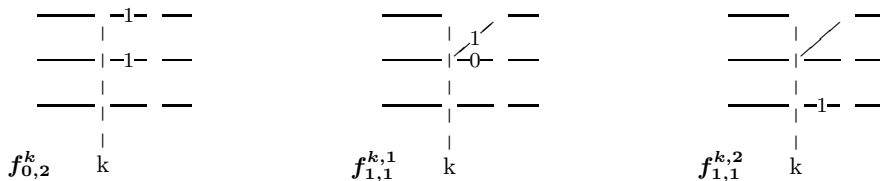
The corresponding measures are given by

$$\Delta_{z,\mathbf{f}_{2,0}^{k,1}}^{(q)} = \eta_n^{\otimes(q-3)} \otimes \left[ \int \eta_k(dw) (\delta_w \overline{Q}_{k,n})^{\otimes 3} \right]$$

$$\Delta_{z,\mathbf{f}_{2,0}^{k,2}}^{(q)}(F) = \eta_n^{\otimes(q-4)} \otimes \left\{ \int \eta_k(dw_1) \eta_k(dw_2) [(\delta_{w_1} \overline{Q}_{k,n})^{\otimes 2} \otimes (\delta_{w_2} \overline{Q}_{k,n})^{\otimes 2}] \right\} \quad (4.16)$$

and we have  $\#(\mathbf{f}_{2,0}^{k,1}) = (q!)^{n+2}/((q-3)!3!)$ , and  $\#(\mathbf{f}_{2,0}^{k,2}) = (q!)^{n+2}/((q-4)!2^3)$ .

There is also a single non coalescent forest  $\mathbf{f}_{0,2}^k$  with two trivial infected trees at level  $k$ . There are two forests  $\mathbf{f}_{1,1}^{k,i}$ ,  $i = 1, 2$ , with one infection and one coalescence at level  $k$ . The first one has a single coalescent tree with only one infected leaf. The last one has a non infected coalescent tree and a single infected trivial tree.

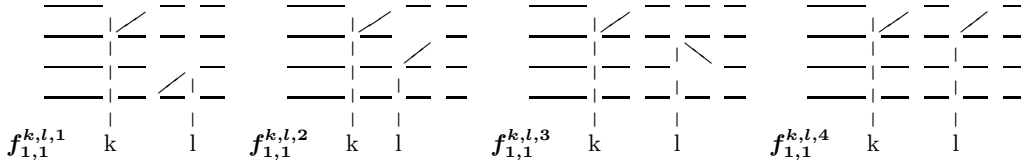


The corresponding measures are given by

$$\begin{aligned}\Delta_{z, \mathbf{f}_{0,2}^{k,1}}^{(q)} &= \eta_n^{\otimes(q-2)} \otimes (\delta_{z_k} \overline{Q}_{k,n})^{\otimes 2} & \Delta_{z, \mathbf{f}_{1,1}^{k,1}}^{(q)} &= \Delta_{z,n, \mathbf{f}_{0,1}^k}^{(q)} \\ \Delta_{z, \mathbf{f}_{1,1}^{k,2}}^{(q)} &= \eta_n^{\otimes(q-3)} \otimes \left[ \int \eta_k(dw) (\delta_w \overline{Q}_{k,n})^{\otimes 2} \right] \otimes (\delta_{z_k} \overline{Q}_{k,n})\end{aligned}\quad (4.17)$$

One checks that  $\#(\mathbf{f}_{0,2}^k) = q^{l^{n+1}} q(q-1)/2$ ,  $\#(\mathbf{f}_{1,1}^{k,1}) = q^{l^{n+1}} q(q-1)$  and  $\#(\mathbf{f}_{1,1}^{k,2}) = \frac{(q!)^{n+2}}{2(q-3)!}$ .

We also have the traditional four non infected forests  $\mathbf{f}_{1,1}^{k,l,i}$ ,  $i = 1, 2, 3, 4$  with two coalescences at level  $k$  and  $l$  [22]. The first one has two coalescent trees with all the leaves at level  $n$ . The second one also has two coalescent trees but one has two leaves at level  $n$ , the other has a leaf at level  $l$  and another at level  $n$ . The third one has a single coalescent tree with three leaves at level  $n$ , and a coalescent branch at level  $l$ . The last one has a single coalescent tree with two leaves at level  $n$  and a coalescent branch at level  $l$ .



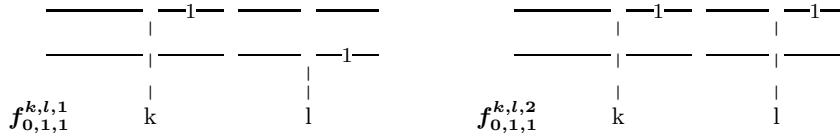
In this case, we readily check that

$$\#(\mathbf{f}_{1,1}^{k,l,1}) = \frac{q^{l^{n+2}}}{4(q-4)!} \quad \#(\mathbf{f}_{1,1}^{k,l,2}) = \frac{q^{l^{n+2}}}{(q-3)!2!} \quad \#(\mathbf{f}_{1,1}^{k,l,3}) = \frac{q^{l^{n+2}}}{(q-3)!2!} \quad \#(\mathbf{f}_{1,1}^{k,l,4}) = \frac{q^{l^{n+2}}}{(q-2)!2!}$$

and the corresponding measures are given by

$$\begin{aligned}\Delta_{z, \mathbf{f}_{1,1}^{k,l,1}}^{(q)} &= \eta_n^{\otimes(q-4)} \otimes \left[ \int \eta_k(du) (\delta_u \overline{Q}_{k,n})^{\otimes 2} \right] \otimes \left[ \int \eta_l(dv) (\delta_v \overline{Q}_{l,n})^{\otimes 2} \right] \\ \Delta_{z, \mathbf{f}_{1,1}^{k,l,2}}^{(q)} &= \eta_n^{\otimes(q-3)} \otimes \left[ \int \eta_k(du) \overline{Q}_{k,l}(1)(u) \delta_u \overline{Q}_{k,n} \right] \otimes \left[ \int \eta_l(dv) (\delta_v \overline{Q}_{l,n})^{\otimes 2} \right] \\ \Delta_{z, \mathbf{f}_{1,1}^{k,l,3}}^{(q)} &= \eta_n^{\otimes(q-3)} \otimes \left[ \int \eta_k(du) \left( \left\{ \int \overline{Q}_{k,l}(u, dv) (\delta_v \overline{Q}_{l,n})^{\otimes 2} \right\} \otimes \delta_u \overline{Q}_{k,n} \right) \right] \\ \Delta_{z, \mathbf{f}_{1,1}^{k,l,4}}^{(q)} &= \eta_n^{\otimes(q-2)} \otimes \left[ \int \eta_k(du) \overline{Q}_{k,l}(1)(u) \overline{Q}_{k,l}(u, dv) (\delta_v \overline{Q}_{l,n})^{\otimes 2} \right]\end{aligned}\quad (4.18)$$

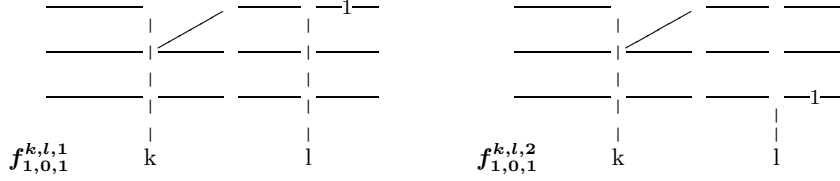
We also have two non coalescent forests  $\mathbf{f}_{0,1,1}^{k,l,i}$ ,  $i = 1, 2$ , with two infections at level  $k$  and  $l$ . The first one has two infected trivial trees. The second one has a trivial tree with two infections.



In this case, we have  $\#(\mathbf{f}_{0,1,1}^{k,l,1}) = q^{l^{n+1}} q(q-1)$  and  $\#(\mathbf{f}_{0,1,1}^{k,l,2}) = q^{l^{n+1}} q$ , and

$$\Delta_{z, \mathbf{f}_{0,1,1}^{k,l,1}}^{(q)} = \eta_n^{\otimes(q-2)} \otimes \delta_{z_k} \overline{Q}_{k,n} \otimes \delta_{z_l} \overline{Q}_{l,n} \quad \text{and} \quad \Delta_{z, \mathbf{f}_{0,1,1}^{k,l,2}}^{(q)} = \overline{Q}_{k,l}(1)(z_k) \left[ \eta_n^{\otimes(q-1)} \otimes \delta_{z_l} \overline{Q}_{l,n} \right]\quad (4.19)$$

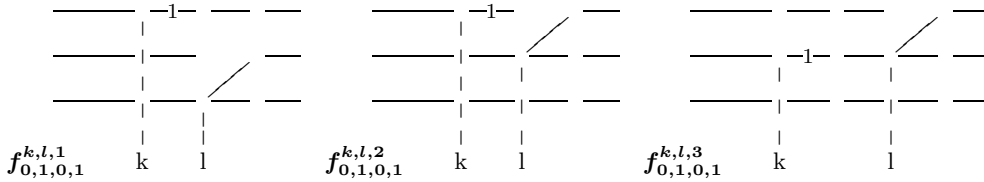
We also have two forests  $\mathbf{f}_{1,0,1}^{k,l,i}$ ,  $i = 1, 2$ , with a coalescence at level  $k$  and an infection at level  $l > k$ . The first one has a coalescent tree with an infection. The second one has a non infected coalescent tree and an infected trivial tree.



In this case we have  $\#(\mathbf{f}_{1,0,1}^{k,l,1}) = q^{l^{n+2}}/(q-2)!$ , and  $\#(\mathbf{f}_{1,0,1}^{k,l,2}) = q^{l^{n+2}}/(2(q-3)!)$ . The corresponding measures are given by

$$\begin{aligned}\Delta_{z, \mathbf{f}_{1,0,1}^{k,l,1}}^{(q)} &= \eta_n^{\otimes(q-2)} \otimes \left[ \int \eta_k(du) \overline{Q}_{k,l}(1)(u) \delta_u \overline{Q}_{k,n} \right] \otimes \delta_{z_l} \overline{Q}_{l,n} \\ \Delta_{z, \mathbf{f}_{1,0,1}^{k,l,2}}^{(q)} &= \eta_n^{\otimes(q-3)} \otimes \left[ \int \eta_k(du) (\delta_u \overline{Q}_{k,n})^{\otimes 2} \right] \otimes \delta_{z_l} \overline{Q}_{l,n}\end{aligned}\quad (4.20)$$

Finally, there are three forests  $\mathbf{f}_{0,1,0,1}^{k,l,i}$ ,  $i = 1, 2, 3$ , with an infection at  $k$  and a coalescence at level  $l > k$ . The first one has a infected tree with a leaf at level  $n$  and a non infected coalescent tree. The second one has a infected tree with a leaf at level  $l$  and a non infected coalescent tree. And finally, the last one has an infected coalescent tree.



In this case we have  $\#(\mathbf{f}_{0,1,0,1}^{k,l,1}) = q^{l^{n+2}}/(2(q-3)!)$  and for any  $i \in \{2, 3\}$   $\#(\mathbf{f}_{0,1,0,1}^{k,l,i}) = q^{l^{n+2}}/(2(q-2)!)$ . In addition, the corresponding measures are given by

$$\begin{aligned}\Delta_{z, \mathbf{f}_{0,1,0,1}^{k,l,1}}^{(q)} &= \eta_n^{\otimes(q-3)} \otimes \left[ \int \eta_l(du) (\delta_u \overline{Q}_{l,n})^{\otimes 2} \right] \otimes \delta_{z_k} \overline{Q}_{k,n} \\ \Delta_{z, \mathbf{f}_{0,1,0,1}^{k,l,2}}^{(q)} &= \overline{Q}_{k,l}(1)(z_k) \left[ \eta_n^{\otimes(q-2)} \otimes \left\{ \int \eta_l(du) (\delta_u \overline{Q}_{l,n})^{\otimes 2} \right\} \right] \\ \Delta_{z, \mathbf{f}_{0,1,0,1}^{k,l,3}}^{(q)} &= \eta_n^{\otimes(q-2)} \otimes \left[ \int \overline{Q}_{k,l}(z_k, du) (\delta_u \overline{Q}_{l,n})^{\otimes 2} \right]\end{aligned}\quad (4.21)$$

For any multi-index  $\boldsymbol{\kappa}$ , and any integer  $i$  we set

$$\overline{\Delta}_{z, \mathbf{f}_{\boldsymbol{\kappa}}^{\dots, i}}^{(q)} := \sum_{0 \leq k < l \leq n} \overline{\Delta}_{z, \mathbf{f}_{\boldsymbol{\kappa}}^{k,l,i}}^{(q)} \quad \text{with} \quad \overline{\Delta}_{z, n, \mathbf{f}_{\boldsymbol{\kappa}}^{k,l,i}}^{(q)} := \Delta_{z, n, \mathbf{f}_{\boldsymbol{\kappa}}^{k,l,i}}^{(q)} - \eta_n^{\otimes q}$$

#### 4.4.5 First and second derivatives

To describe with some precision the first two order derivatives of the mapping  $N \mapsto \Upsilon_{z,n}^{(q)}$  we need to compute the expectation operators on random infected forests defined in (4.14). The ones associated with forests with at most one infection or one coalescence at some level only depend on one class of forests. Thus, using (4.15) their description is immediate. Using (4.16), the centered operator associated with non infected forests with a couple of coalescence at some level is given by

$$\overline{\Delta}_{z, \mathbf{f}_{2,0}^{\dots, \star}}^{(q)} := \frac{1}{1 + \frac{3}{4}(q-3)} \overline{\Delta}_{z, \mathbf{f}_{2,0}^{\dots, 1}}^{(q)} + \left( 1 - \frac{1}{1 + \frac{3}{4}(q-3)} \right) \overline{\Delta}_{z, \mathbf{f}_{2,0}^{\dots, 2}}^{(q)}$$



In much the same way, by (4.17) the one associated with forests with a single coalescence and a single infection at some level is given by

$$\overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, \star}}^{(q)} := \frac{2}{q} \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, 1}}^{(q)} + \left(1 - \frac{2}{q}\right) \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, 2}}^{(q)}$$

In view of (4.18), the centered expectation operator associated with forests with a single coalescence at two different levels is given by

$$\begin{aligned} \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, \star}}^{(q)} &:= \frac{(q-2)(q-3)}{(q-2)(q-3) + 4(q-2) + 2} \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, 1}}^{(q)} \\ &\quad + \frac{2(q-2)}{(q-2)(q-3) + 4(q-2) + 2} \left[ \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, 2}}^{(q)} + \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, 3}}^{(q)} \right] \\ &\quad + \frac{2}{(q-2)(q-3) + 4(q-2) + 2} \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, 4}}^{(q)} \end{aligned}$$

Using (4.19) the one associated with non coalescent forests with a single infection at two different levels is given by

$$\overline{\Delta}_{z, \mathbf{f}_{0,1,1}^{\bullet, \star}}^{(q)} := \left(1 - \frac{1}{q}\right) \overline{\Delta}_{z, \mathbf{f}_{0,1,1}^{\bullet, 1}}^{(q)} + \frac{1}{q} \overline{\Delta}_{z, \mathbf{f}_{0,1,1}^{\bullet, 2}}^{(q)}$$

Finally, using (4.20) and (4.21) the operator associated with a single coalescence and a single infection at two different levels are given by

$$\overline{\Delta}_{z, \mathbf{f}_{1,0,1}^{\bullet, \star}}^{(q)} := \frac{2}{q} \overline{\Delta}_{z, \mathbf{f}_{1,0,1}^{\bullet, 1}}^{(q)} + \left(1 - \frac{2}{q}\right) \overline{\Delta}_{z, \mathbf{f}_{1,0,1}^{\bullet, 2}}^{(q)}$$

and

$$\overline{\Delta}_{z, \mathbf{f}_{0,1,0,1}^{\bullet, \star}}^{(q)} := \left(1 - \frac{2}{q}\right) \overline{\Delta}_{z, \mathbf{f}_{0,1,0,1}^{\bullet, 1}}^{(q)} + \frac{1}{q} \overline{\Delta}_{z, \mathbf{f}_{0,1,0,1}^{\bullet, 2}}^{(q)} + \frac{1}{q} \overline{\Delta}_{z, \mathbf{f}_{0,1,0,1}^{\bullet, 3}}^{(q)}$$

Expanding the formulae stated in theorem 4.23, extending the combinatorial methods developed in [22] for computing the cardinals  $\#(\mathbf{f})$  we prove the following expansions.

**Corollary 4.24** *The first three derivatives of  $\Upsilon_{z,n}^{(N,q)}$  are given by*

$$\begin{aligned} d^{(0)} \Upsilon_{z,n}^{(q)} &= \eta_n^{\otimes q} \\ d^{(1)} \Upsilon_{z,n}^{(q)} &= \tau_{q,1,0}^{(1)} \overline{\Delta}_{z, \mathbf{f}_{1,0}^{\bullet}}^{(q)} + \tau_{q,0,1}^{(1)} \overline{\Delta}_{z, \mathbf{f}_{0,1}^{\bullet}}^{(q)} \\ d^{(2)} \Upsilon_{z,n}^{(q)} &= \tau_{q,1,0}^{(2)} \overline{\Delta}_{z, \mathbf{f}_{1,0}^{\bullet}}^{(q)} + \tau_{q,0,1}^{(2)} \overline{\Delta}_{z, \mathbf{f}_{0,1}^{\bullet}}^{(q)} + \tau_{q,1,1}^{(2)} \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, \star}}^{(q)} + \tau_{q,2,0}^{(2)} \overline{\Delta}_{z, \mathbf{f}_{2,0}^{\bullet, \star}}^{(q)} + \tau_{q,0,2}^{(2)} \overline{\Delta}_{z, \mathbf{f}_{0,2}^{\bullet}}^{(q)} \\ &\quad + \left(\tau_{q,1,0}^{(1)}\right)^2 \overline{\Delta}_{z, \mathbf{f}_{1,1}^{\bullet, \star}}^{(q)} + \left(\tau_{q,0,1}^{(1)}\right)^2 \overline{\Delta}_{z, \mathbf{f}_{0,1,1}^{\bullet, \star}}^{(q)} + \tau_{q,1,0}^{(1)} \tau_{q,0,1}^{(1)} \left\{ \overline{\Delta}_{z, \mathbf{f}_{1,0,1}^{\bullet, \star}}^{(q)} + \overline{\Delta}_{z, \mathbf{f}_{0,1,0,1}^{\bullet, \star}}^{(q)} \right\} \\ &\quad + n \tau_{q,0,0}^{(1)} \left[ \tau_{q,1,0}^{(1)} \overline{\Delta}_{z, \mathbf{f}_{1,0}^{\bullet}}^{(q)} + \tau_{q,0,1}^{(1)} \overline{\Delta}_{z, \mathbf{f}_{0,1}^{\bullet}}^{(q)} \right] \end{aligned}$$

with the parameters  $\tau_{q,p_1,p_2}^{(m)}$  given in (4.4).

When  $q = 1$ , all the terms are null except  $\tau_{1,0,1}^{(1)} = 1 = -\tau_{1,0,0}^{(1)}$ . In this case, we find that

$$\begin{aligned} d^{(1)}\Upsilon_{z,n}^{(1)} &= \sum_{0 \leq k \leq n} \left[ \Delta_{z, \mathbf{f}_{\mathbf{0},1}^k}^{(1)} - \eta_n \right] = \sum_{0 \leq k \leq n} \delta_{z_k} (\bar{Q}_{k,n} - \eta_n) \\ d^{(2)}\Upsilon_{z,n}^{(1)} &= \bar{\Delta}_{z, \mathbf{f}_{\mathbf{0},1,1}^{1,2}}^{(1)} - n \bar{\Delta}_{z, \mathbf{f}_{\mathbf{0},1}^{(1)}} \\ &= \sum_{0 \leq k < l \leq n} [\bar{Q}_{k,l}(1)(z_k) \delta_{z_l} \bar{Q}_{l,n} - \eta_n] - n \sum_{0 \leq k \leq n} [\delta_{z_k} \bar{Q}_{k,n} - \eta_n] \end{aligned}$$

## 5 Some extensions and open questions

### 5.1 Island type methodologies

Particle MCMC methods are computationally intensive sampling techniques. As discussed in [28, 46], parallel and distributed computations provide an appealing solution to tackle these issues. The central idea of Island models is run in parallel  $N_2$  particle models with  $N_1$  individuals, instead of running a single particle model with  $N_1 N_2$  particles. These  $N_2$  batches are termed islands in reference to dynamic population models. Within each island the  $N_1$  individuals evolve as a standard genetic type particle model. In this interpretation, island particle models can be thought as a parallel implementation of particle models. In the further development of this section, we show that these methodologies can also be used in a natural way to design island type particle MCMC samplers.

To design these models, we consider a collection of bounded and non negative potential functions  $\mathfrak{G}_n$  on some measurable state spaces  $\mathfrak{E}_n$ , with  $n \in \mathbb{N}$ . We let  $\mathfrak{X}_n$  be a Markov chain on  $\mathfrak{E}_n$  with initial distribution  $\mu_0 \in \mathcal{P}(\mathfrak{E}_0)$  and some Markov transitions  $\mathfrak{M}_n$  from  $\mathfrak{E}_{n-1}$  into  $\mathfrak{E}_n$ . The Feynman-Kac measures  $(\mu_n, \nu_n)$  associated with the parameters  $(\mathfrak{G}_n, \mathfrak{M}_n)$  are defined for any  $\mathbf{f}_n \in \mathcal{B}(\mathfrak{E}_n)$  by the formulae

$$\mu_n(\mathbf{f}_n) := \nu_n(\mathbf{f}_n) / \nu_n(1) \quad \text{with} \quad \nu_n(\mathbf{f}_n) := \mathbb{E} \left( \mathbf{f}_n(\mathfrak{X}_n) \prod_{0 \leq p < n} \mathfrak{G}_p(\mathfrak{X}_p) \right) \quad (5.1)$$

The mean field  $N'$ -particle approximation

$$X'_n = (X_n^i)_{1 \leq i \leq N'} \in S'_n := \mathfrak{E}_n^{[N']}$$

of these Feynman-Kac models is defined as in (2.3) by considering the evolution semigroup of the Feynman-Kac model  $\mu_n$ .

We let  $M'_n$  be Markov transitions of  $X'_n$  and we consider the potential functions  $G'_n$  on  $S'_n$  defined by

$$G'_n(X'_n) = m(X'_n)(\mathfrak{G}_n) = \frac{1}{N'} \sum_{1 \leq i \leq N'} \mathfrak{G}_n(X_n^i) \quad (5.2)$$

We let  $(\eta'_n, \gamma'_n)$  be the Feynman-Kac measures associated with the parameters  $(G'_n, M'_n)$ . In this framework, the unbiasedness properties of the unnormalized Feynman-Kac particle measures takes the form

$$\begin{aligned} f'_n(X'_n) &= m(X'_n)(\mathbf{f}_n) \\ \implies \nu_n(\mathbf{f}_n) &= \mathbb{E} \left( \mathbf{f}_n(\mathfrak{X}_n) \prod_{0 \leq p < n} \mathfrak{G}_p(\mathfrak{X}_p) \right) = \mathbb{E} \left( f'_n(X'_n) \prod_{0 \leq p < n} G'_p(X'_p) \right) = \gamma'_n(f'_n) \end{aligned} \quad (5.3)$$

The path space version  $(\eta_n, \gamma_n)$  of these measures are defined by the Feynman-Kac measures associated with the historical process  $X_n$  and the potential function  $G_n$  given by

$$X_n = (X'_0, \dots, X'_n) \in S_n = (S'_0 \times \dots \times S'_n) \quad \text{and} \quad G_n(X_n) = G'_n(X'_n)$$

The mean field  $N$ -particle approximations  $\xi'_n = (\xi'_n)^i_{1 \leq i \leq N}$  of the measures  $(\eta'_n, \gamma'_n)$  can be interpreted as a genetic type model island type particles

$$\forall 1 \leq i \leq N \quad \xi'_n{}^i = (\xi'_n{}^{i,j})_{1 \leq j \leq N'} \in S'_n := \mathfrak{E}_n^{[N']}$$

with mutation transitions  $M'_n$  and the selection potential functions  $G'_n$  given in (5.2). By construction, the  $N$ -particle approximation  $\xi_n$  of the path space measures  $(\eta_n, \gamma_n)$  is an a genealogical tree based model in the space of islands. Each particle

$$\xi_n^i = (\xi_{0,n}^i, \dots, \xi_{n,n}^i) \in S_n = \left( \mathfrak{E}_0^{[N']} \times \dots \times \mathfrak{E}_n^{[N']} \right)$$

represents the line of island ancestor  $\xi_{p,n}^i \in \mathfrak{E}_p^{[N']}$  of the  $i$ -th island  $\xi_{n,n}^i = \xi_n^i \in \mathfrak{E}_n^{[N]}$  at time  $n$ , at every level  $0 \leq p \leq n$ , with  $1 \leq i \leq N$ . In other words,  $(\eta_n, \gamma_n, \xi_n)$  is the historical version of the Feynman-Kac model  $(\gamma'_n, \eta'_n, \xi'_n)$ . In this case, the dual mean field particle model  $\mathcal{X}_n$  evolves on the state spaces  $\mathcal{S}_n = S_n^{[N]}$ , with a frozen trajectory of islands  $X_n$ .

This model can be interpreted as the evolution of  $N$  interacting islands

$$\forall 1 \leq i \leq N \quad \mathcal{X}_n^i = (\mathcal{X}_n^{i,j})_{1 \leq j \leq N'} \in \mathfrak{E}_n^{[N']}$$

with  $N'$  individuals in each island. The conditional particle Markov chain models discussed in section 3.3 can be used without further work to design island type particle Markov chain models with the target measure  $\eta_n$ . Using (5.3), we see that the  $S'_n$ -marginal of  $\eta_n$  can be used to compute any Feynman measures of the form (5.1). Similar constructions can be developed to design a backward-sampling based particle MCMC model.

Of course, we can iterate these Russian nesting doll type constructions at any level. For a more thorough discussion on these island type particle methodologies we refer the reader to [20, 21], and the recent article [46].

## 5.2 Some open problems

This paragraph is dedicated at stating some important open questions related to conditional particle MCMC models.

The first one is to find a Taylor type expansion of the backward sampling based Markov transition  $\mathbb{K}_n$  around its invariant measure  $\eta_n$  w.r.t. powers of  $1/N$ . One possible route is to develop Taylor type expansions of the tensor product of the unbiased particle model  $\gamma_n^{(N,2)}$  introduced in (2.8). Whenever they exist, these expansions could be extended to particle models with a frozen trajectory. The analogous problem for  $\mathbb{K}_n$  has been addressed in the present paper, see Fla (3.12).

Another important problem is to compare the contraction properties of the couple of conditional PMCMC models discussed in section section 3.3. Some comparisons based on coupling and one step transition minorization techniques have been developed by the articles [4, 9, 34]. Another natural strategy would be to compare (whenever they exist) the Taylor expansions of the iterates of PMCMC transitions –this is one of the motivations for deriving Taylor expansions for these transitions.

At last, a third important question is to analyze the convergence properties of the islands type particle models presented above in terms of the number of individual and the number of islands.

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