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Doi–Peliti path integral methods for stochastic systems with partial exclusion

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HIGHLIGHTS

- Doi–Peliti methods for stochastic models with partial exclusion.
- Paragrassmannian path integral actions constructed with the aid of Magnus expansions.
- Carrying capacity birth–death processes have exact perturbative expansions.

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ABSTRACT

Doi–Peliti methods are developed for stochastic models with finite maximum occupation numbers per site. We provide a generalized framework for the different Fock spaces reported in the literature. Paragrassmannian techniques are then utilized to construct path integral formulations of factorial moments. We show that for many models of interest, a Magnus expansion is required to construct a suitable action, meaning actions containing a finite number of terms are not always feasible. However, for such systems, perturbative techniques are still viable, and for some examples, including carrying capacity population dynamics, and diffusion with partial exclusion, the expansions are exactly summable.

1. Introduction

This work is concerned with parallels between quantum field theory (QFT) and population dynamics. QFT was developed [1,2] to model interactions of subatomic particles. These interactions result in particle populations that vary in size and position. Classical population dynamics also model populations that vary in size, via mechanisms such as birth–death processes, for example. These populations can also vary in 'position', where position can be interpreted as a continuous feature of interest, such as physical location of a molecule, the size of a cell, or the age of individuals, for example. Doi [3,4] was the first to notice this parallel and used QFT machinery to model molecular reactions.

The path integral formulation of quantum mechanics was introduced by Dirac, further developed and popularized by Feynman [5]. Peliti [6] adapted these ideas, using functional integration techniques to construct path integral formulations of the Doi paradigm. These techniques have seen a range of applications including molecular reactions [3,4], birth–death processes on lattices [6,7], branching random walks [8], percolation [9], phylogenetics [10], algebraic probability [11], knot theory [12], and age dependent population dynamics [13], to name a few.

These works have all been concerned with bosonic forms of QFT, applied to systems with no restriction in occupation number. It is natural to consider analogous applications of fermionic QFT, used to describe quantum systems where there can be no more than one particle in a given state. These techniques can be adapted to population dynamics by modeling

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classical motions of particles on a lattice, where each site is exclusive, being restricted to single maximum occupancy. Such an approach has been successfully used to model a range of systems such as aggregation processes [14], Ising models [15], and lattice diffusion [16], for example. Exclusive dynamics have also been achieved within a bosonic framework [17]. Grassmannian path integral techniques can also be adapted to such systems [18,19].

In addition to bosonic (unrestricted) and fermionic (single occupancy) statistics, QFT has been developed for states with limited occupation number. This was first developed by Green [20] and has since been well characterized with the aid of generalized paragrassmannian variables [21], although no fundamental particles of this nature have been observed to date, and path integral formulations for these methods are not widespread [22,23]. The Doi framework using parafermi QFT techniques for stochastic systems with partial exclusion has developed for cyclic chemical reactions [24], and for diffusion [25,26], although path integral techniques have not previously been considered. We turn to this problem and address this deficit with the work presented.

We also mention that significant work in renormalization with Doi–Peliti techniques have also been developed [7,27,28,8,29,30], although such methods are not explored in this work. A recent review of Doi–Peliti approaches can be found in [31].

The systems that we shall apply these methods to are partially excluded lattice diffusion [26,25,16], where maximum particle numbers are fixed over a lattice of sites, and birth–death processes with a carrying capacity, where population size is limited over a single site. The term carrying capacity usually refers to biological species, representing the maximum population size that can be supported given the available resources (e.g. food, space, competition etc.). Such birth–death processes are also known as stochastic logistic growth or Verhulst models [32,33], and are characterized by birth and death rates β_n and μ_n which depend upon population size n in some capacity limiting fashion. A linear birth rate $\beta_n = p - n$, for example, reduces as the population capacity p is approached. Such linear systems can be analyzed using classical techniques [34,35]. However, the per individual rate $\frac{\beta_n}{n} = \frac{p}{n} - 1$ is not very natural. A birth rate $\beta_n = n(p-n)$ has a linear per individual birth rate, and approaches zero as full capacity is reached. Although more natural, the quadratic nature makes this difficult to analyze analytically [34,36]. A death rate $\mu_n = \mu n$ has a constant death rate per individual, and approaches zero as the population empties, so is reasonably natural and the approach we take, although quadratic death rates could similarly be considered.

The work is organized as follows. Section 2 develops a generalized Fock system suitable for stochastic systems with partial exclusion, explaining the different Fock spaces found in the literature [25,24,26]. Section 3 describes how generalized paragrassmannian algebras can be used to construct coherent states. Section 4 develops a coherent state path integral representation, demonstrating that the non-commutative nature of paragrassmannian variables means Magnus expansions [37,38] are required to construct path integral actions. Section 5 considers applications to birth–death processes and diffusion. Conclusions in Section 6 complete the work.

2. Fock spaces

2.1. General structure

We assume in all that follows that the maximum occupancy of any site is p. We also assume, until otherwise stated, that we are dealing with a single site, with occupancy n. We let a and $a^\dagger$ represent annihilation and creation operators for a single site. The Green parafermi relations then take the form [20,21]

$$[a, [a^\dagger, a]] = 2a. \tag{1}$$

When Green introduced parastatistics, he used what is now referred to as the Green representation. In this formulation we have p distinct occupational 'bins', the ith associated with standard Pauli operators a_i and $a_i^\dagger$. These obey standard anti-commutation relations

$$\{a_i, a_i^\dagger\} = 1, \qquad \{a_i, a_i\} = \{a_i^\dagger, a_i^\dagger\} = 0. \tag{2}$$

These operators commute for distinct i, j, so $[a_i, a_j^\dagger] = 0$, for example. One can then show that operator $a = \sum_i a_i$ satisfies the Green relation of Eq. (1).

Next we introduce states $|n\rangle$ with $n \in \{0, 1, \ldots, p\}$ such that

$$a^\dagger|n\rangle = p_n|n+1\rangle, \qquad a|n\rangle = q_n|n-1\rangle, \tag{3}$$

where p_n, q_n are normalization factors that will later be specified. Repeated application of these recurrences results in

$$|n\rangle = \frac{(a^\dagger)^n}{\prod_{i=0}^{n-1} p_i}|0\rangle, \qquad a^n|n\rangle = \prod_{i=1}^{n} q_i|0\rangle. \tag{4}$$

Now, the commutation relations can be applied to show that $a^n(a^\dagger)^n|0\rangle = (n!)^2\binom{p}{n}|0\rangle$. We thus find from Eq. (4) that $(n!)^2\binom{p}{n} = \prod_{i=1}^{n} p_{i-1}q_i$, which results in the expression

$$p_{n-1}q_n = n(p-n+1). \tag{5}$$