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LETTER TO THE EDITOR

Equivalence between Poisson representation and Fock space formalism for birth–death processes

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Abstract. The equivalence between the Poisson representation and the Fock space formalism, both used to derive coarse-grained equations from the master equation for non-equilibrium systems, is explicitly demonstrated.

In statistical mechanics, the dynamics of a system near or at equilibrium can be described at different levels. At a microscopic level the dynamics is given by a master equation governing the time evolution of the probability that a microscopic state is realized at a given time t. At a coarsed-grained level, the dynamics is described by one (or a few coupled) Langevin equations. When the system evolves towards an equilibrium state, the noise is usually additive and white, and in this case an alternative description exists in terms of a Fokker–Planck equation [1]. In many situations, a mean-field like approximation, neglecting the fluctuations, already gives a correct description of most of the properties of the system. However, this is obviously not true in the vicinity of a phase transition [2].

For non-equilibrium systems, the situation is often more subtle. For example, the system can evolve towards an empty state (for which no particles are left in the system). One can then expect that, in the long time regime, the fluctuations will govern the dynamics. Examples are provided by reaction-diffusion systems, of which the simplest is the annihilation model in which A particles diffuse in a gel and annihilate [3] according to:

$$A + A \to \emptyset. \tag{1}$$

For a d-dimensional system and homogeneous initial conditions, $n_A(t)$, the number of particles at time t, behaves in the long time regime as $n_A(t) \sim t^{-\alpha}$, where $\alpha = \min(1, d/2)$. One speaks of anomalous kinetics. Indeed, a simple mean-field description (rate equation) predicts $\alpha = 1$ in all dimensions. Similar situations happen in more complicated reactions of the type $nA + mB \to C$ [4]. In this case one can also consider situations in which the particles A and B are initially separated in space. Reaction-diffusion fronts are then formed with non-trivial dynamical scaling properties [5].

To describe these non-equilibrium situations, one has to start at the master equation level to keep track of all the fluctuations. However, scaling behaviour usually takes place in the

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long time regime. It is thus natural to seek a coarse-grained theory which can be analysed in the framework of a dynamical renormalization group, for example. It is, however, crucial that this coarse-grained theory keeps track of all the important fluctuations contained in the system.

Two different approaches, apparently disconnected one from the other, have been proposed in the literature: the Fock space formalism [6] and the Poisson representation [7]. The purpose of this note is to show explicitly that, although starting from a different point of view, the two above approaches are equivalent. Namely, there is a one to one correspondence between the Liouvillians and the field theories of the two methods.

Let us first consider a zero dimensional system. The generalization to arbitrary dimensions is straightforward, but the notation becomes cumbersome. One considers a dynamical process described by the following master equation:

$$\partial_t \phi_n(t) = \sum_{n' \neq n} [w(n' \to n)\phi_{n'}(t) - w(n \to n')\phi_n(t)] \tag{2}$$

where $\phi_n(t)$ is the probability that the system has n particles at time t and $w(n' \to n)$ is the transition rate from the state with n' particles to the one with n particles.

In the approach using the Fock space formalism [6], one introduces creation and annihilation operators in a way similar to quantum theory. To each macroscopic state $\{\phi_n\}$ one can associate the state $|\Phi\rangle$ considered as an element of a real vector space or a Fock space $\mathcal{F}$ [8]:

$$|\Phi\rangle = \sum_n \phi_n |n\rangle \tag{3}$$

where $|n\rangle$ is the state with exactly n particles. A useful quantity is the generating function defined as:

$$G(z, t) = \sum_n \phi_n(t) z^n \tag{4}$$

where z is a complex number. The derivatives of $G(z, t)$ generate the factorial moments:

$$n_k(\phi) = \langle n(n-1)\dots(n-k+1)\rangle = \frac{\partial^k}{\partial z^k} G(z, t)|_{z=1}. \tag{5}$$

The definition of a scalar product on the vector space gives it a Hilbert structure. Two different scalar products are usually considered [9, 10]. For simplicity we shall restrict ourselves to the so-called exclusive scalar product defined as:

$$\langle n|m\rangle = n!\delta_{nm}. \tag{6}$$

One then introduces the annihilation operator a and the creation operator π defined as:

$$a|n\rangle = n|n-1\rangle \tag{7}$$

and

$$\pi|n\rangle = |n+1\rangle. \tag{8}$$

These operators obey the usual commutations relations:

$$[a, \pi]_- = 1 \tag{9}$$

and are Hermitian conjugates with respect to the exclusive scalar product. It then follows that:

$$\phi_n(t) = \frac{1}{n!}\langle n|\Phi\rangle = \frac{1}{n!}\langle 0|a^n|\Phi(t)\rangle. \tag{10}$$

Finally, the generating function can be written down in this formalism as:

$$G(z, t) = \langle z|\Phi\rangle \tag{11}$$

where the $|z\rangle$ are the coherent states of Bargmann and Fock [11]:

$$|z\rangle = \exp(z^*\pi)|0\rangle. \tag{12}$$

One can then prove several useful properties:

$$\langle z|\zeta\rangle = e^{z\zeta^*} \tag{13}$$

$$\int \frac{dz\, dz^*}{2\pi i} e^{-zz^*}|z\rangle\langle z| = I \tag{14}$$

$$|\Phi\rangle = \int \frac{dz\, dz^*}{2\pi i} e^{-zz^*} G(z, t)|z\rangle \tag{15}$$

$$a|z\rangle = z^*|z\rangle. \tag{16}$$

In this approach the master equation takes the form:

$$\partial_t|\Phi\rangle = \mathcal{L}^{\mathcal{F}}|\Phi\rangle \tag{17}$$

with the Liouvillian $\mathcal{L}^{\mathcal{F}}$ being a polynomial in the creation and annihilation operators and can always be written in normal form (all the creation operators are on the left of the annihilation operators):

$$\mathcal{L}^{\mathcal{F}} = \sum_{i,j} C_{ij}\pi^i a^j. \tag{18}$$

The exact form of $\mathcal{L}^{\mathcal{F}}$, i.e. the values that the constants C_{ij} take on, will depend on the form of the transition rates $w(n' \to n)$ for the model under consideration. Thus one can take either the w or the Liouvillian $\mathcal{L}^{\mathcal{F}}$ to define the model.

From (17) and (18) one can construct a path-integral representation for

$$P(z, t|z_0, 0) = \langle z|\exp t\mathcal{L}^{\mathcal{F}}|z_0\rangle \tag{19}$$

by inserting (14) into (19) $N-1$ times, in the usual way [11]:

$$P(z, t|z_0, 0) = \left(\prod_{k=1}^{N-1}\int \frac{dz_k\, dz_k^*}{2\pi i} e^{-z_k z_k^*}\right)\langle z_N|\exp\epsilon\mathcal{L}^{\mathcal{F}}|z_{N-1}\rangle \cdot \langle z_{N-1}|\exp\epsilon\mathcal{L}^{\mathcal{F}}|z_{N-2}\rangle$$
$$\ldots\langle z_1|\exp\epsilon\mathcal{L}^{\mathcal{F}}|z_0\rangle \tag{20}$$

where $z_N = z$ and where $\epsilon = t/N$. For small ϵ a typical term may easily be evaluated:

$$\langle z_k | \exp \epsilon \mathcal{L}^{\mathcal{F}} | z_{k-1} \rangle \sim \exp\left(\epsilon \sum_{i,j} C_{ij} z_k^i (z_{k-1}^*)^j + z_k z_{k-1}^* \right). \tag{21}$$

Substituting (21) into (20) and taking the limit $N \to \infty$ and $\epsilon \to 0$ with t fixed, gives for (20), after some algebra and up to boundary terms:

$$\int \mathrm{d}[z, z^*] \exp - \left\{ \int_0^t \mathrm{d}t \, [z\dot{z}^* - \sum_{i,j} C_{ij} z^i (z^*)^j] \right\} \tag{22}$$

where the dot signifies differentiation with respect to time. This is essentially the form given in [8] and can be used as the basis for approximation schemes in these systems.

There is, however, a different method available which starts from a master equation such as (2) and leads, also without approximation, to a path-integral representation for the process. The method uses the Poisson representation, and was introduced by Gardiner and Chaturvedi [7] and developed by Elderfield [12]. Specifically one assumes that a state of the system realised at time t can be expanded as a superposition of multivariate uncorrelated Poissons. One then writes:

$$\phi_n(t) = \int \mathrm{d}\alpha \, \frac{(\exp -\alpha)\alpha^n}{n!} f(\alpha, t). \tag{23}$$

In this formalism the generating function, (4), takes the form:

$$G(z, t) = \int \mathrm{d}\alpha \, \exp[(z-1)\alpha] f(\alpha, t). \tag{24}$$

If one is given the evolution equation for G in the form

$$\partial_t G(z, t) = \mathcal{L}^{\mathcal{G}} G(z, t) \tag{25}$$

then by replacing G by its expression (24), and integrating by parts (assuming that $f(\alpha, t)$ and some of its derivatives vanish at the boundaries) one obtains a Fokker–Planck-like equation for $f(\alpha, t)$ [1, 7]. This equation is not a standard Fokker–Planck equation because $f(\alpha, t)$ does not have to remain positive and thus is not a probability density. Moreover, α is not necessarily real, but can be complex. This Poisson representation leads to simple relations between the factorial moments of n and the moments of α. One has:

$$n_k(f) = \int \mathrm{d}\alpha \, \alpha^k f(\alpha, t) = \langle \alpha^k \rangle. \tag{26}$$

To show the equivalence of the two formalisms, one has first to determine the form of the Liouvillian, $\mathcal{L}^{\mathcal{G}}$, defined in (25), which describes the evolution of the generating function, $G(z, t)$, with time. Given the form (18) for $\mathcal{L}^{\mathcal{F}}$ this is straightforward:

$$\begin{aligned} \partial_t G(z, t) &= \langle z | \partial_t | \Phi \rangle \\ &= \langle z | \mathcal{L}^{\mathcal{F}} | \Phi \rangle \\ &= \sum_{ij} C_{ij} \int \frac{\mathrm{d}\zeta \mathrm{d}\zeta^*}{2\pi i} \mathrm{e}^{-\zeta\zeta^*} G(\zeta, t) \langle z | \pi^i a^j | \zeta \rangle \end{aligned} \tag{27}$$

where we have used (15). Now using (13) and (16) one has

$$\partial_t G(z,t) = \sum_{i,j} C_{ij} z^i \left(\frac{\partial}{\partial z}\right)^j (z|\Phi) = \mathcal{L}^{\mathcal{G}} G(z,t) \tag{28}$$

where

$$\mathcal{L}^{\mathcal{G}} = \sum_{i,j} C_{ij} z^i \left(\frac{\partial}{\partial z}\right)^j. \tag{29}$$

One sees the close relationship between $\mathcal{L}^{\mathcal{F}}$ and $\mathcal{L}^{\mathcal{G}}$. To each creation operator π present in $\mathcal{L}^{\mathcal{F}}$ one associates a factor z in $\mathcal{L}^{\mathcal{G}}$ and to each annihilation operator a in $\mathcal{L}^{\mathcal{F}}$ one associates the operator $\partial/\partial z$ in $\mathcal{L}^{\mathcal{G}}$.

It is now possible to proceed from (25) as described above to find the evolution equation for $f(\alpha, t)$. One finds:

$$\partial_t f(\alpha, t) = \mathcal{L}^{\mathcal{P}} f(\alpha, t) \tag{30}$$

where

$$\mathcal{L}^{\mathcal{P}} = \sum_{i,j} C_{ij} \left(1 - \frac{\partial}{\partial \alpha}\right)^i \alpha^j \tag{31}$$

is the Liouvillian describing the evolution of the quasi-probability density $f(\alpha, t)$. This Fokker–Planck-like equation is exact—no approximation or truncation has been made in deriving it from the master equation (2). It can be used as the basis for the study of processes described by (2), or as the starting point for deriving a path-integral representation in terms of the α variables. To carry out this latter programme, one introduces operators $\hat{\alpha}$ and $\hat{p}$ [12] satisfying

$$[\hat{\alpha}, \hat{p}]_- = i \qquad [\hat{\alpha}, \hat{\alpha}]_- = 0 \qquad [\hat{p}, \hat{p}]_- = 0 \tag{32}$$

with

$$\hat{p} = -i \frac{\partial}{\partial \alpha} \tag{33}$$

in the α-representation. Then just as the master equation (17) is the Fock-space analogue of (25), one can write an operator analogue of (31):

$$\partial_t |f\rangle = \mathcal{L}^{\mathcal{O}} |f\rangle \tag{34}$$

where:

$$\mathcal{L}^{\mathcal{O}} = \sum_{i,j} C_{ij} (1 + i\hat{p})^i (\hat{\alpha})^j. \tag{35}$$

Introducing $|\alpha\rangle$ and $|p\rangle$, which are eigenkets of $\hat{\alpha}$ and $\hat{p}$ with eigenvalues α and p respectively, one can derive a path-integral representation for

$$f(\alpha, t|\alpha_0, 0) = \langle \alpha | \exp t\mathcal{L}^{\mathcal{O}} | \alpha_0 \rangle \tag{36}$$

in exactly the same way as described in (19) *et seq.* One finds the analogous expression to (22) to be

$$\int \mathrm{d}[p,\alpha]\,\exp-\left\{\int_0^t \mathrm{d}t\,[ip\dot{\alpha}-\sum_{i,j}C_{ij}(1+ip)^i\alpha^j]\right\}. \tag{37}$$

The 'action' in the path-integral (22) and that in (37) are identical as long as the identifications

$$\alpha \leftrightarrow z^* \qquad ip \leftrightarrow (z-1) \tag{38}$$

are made. Although it was not obvious *a priori* that the two actions would be identical, if (38) is expressed in the form:

$$\alpha \leftrightarrow \frac{\partial}{\partial z} \qquad \frac{\partial}{\partial \alpha} \leftrightarrow (z-1) \tag{39}$$

it becomes very much more plausible, given the conjugate nature of the variables α and $(z-1)$ indicated in (24).

The generalization to d-dimensional systems on a lattice is straightforward [8]. At each site r of the lattice, one can have n_r particles. One starts with a master equation for $\phi_{n_1,n_2,\ldots,n_r,\ldots}(t)$, the joint probability to find n_j particles at site j $(j=1,2,\ldots)$.

In the Fock space representation, the basis states of the system are of the form $|\underline{n}\rangle \equiv |n_1,n_2,\ldots n_r,\ldots\rangle$. At each site r of the lattice, one associates a pair of creation π_r and annihilation a_r operators satisfying the commutation relations:

$$[a_r,\pi_s]_- = \delta_{rs}. \tag{40}$$

The macroscopic state is:

$$|\Phi\rangle = \sum_{\underline{n}} \phi_{\underline{n}}|\underline{n}\rangle \tag{41}$$

and the generating function:

$$G(z_1,z_2,\ldots z_r,\ldots;t) = \sum_{\underline{n}}\prod_r \phi_{\underline{n}} z_r^{n_r}. \tag{42}$$

The Liouvillian $\mathcal{L}^{\mathcal{F}} = \mathcal{L}(\pi_1,a_1,\ldots,\pi_j,a_j,\ldots)$ contains terms which couple the site r and its nearest neighbours. Such non-local terms are needed to describe the diffusion of the particles on the lattice.

In the Poisson representation, one expresses $\phi_{\underline{n}}$ as a multiple integral of the form:

$$\phi_{\underline{n}}(t) = \int \mathrm{d}\underline{\alpha}\prod_r \frac{\alpha_r^{n_r}\exp(-\alpha_r)}{n_r!} f(\underline{\alpha},t) \tag{43}$$

where $\underline{\alpha} = (\alpha_1,\alpha_2,\ldots)$. The generating function becomes:

$$G(\underline{z},t) = \int \mathrm{d}\underline{\alpha}\,\exp\left[\sum_r (z_r-1)\alpha_r\right] f(\underline{\alpha},t). \tag{44}$$

One can now see that to show the equivalence of the two formalisms in the general d-dimensional case, one can proceed in exactly the same way as for the one-site problem. First of all, an analogous procedure to that carried out in (27)–(29) shows that the Liouvillian describing the evolution of $G(\underline{z}, t)$ is $\mathcal{L}^{\mathcal{G}} = \mathcal{L}(z_1, \partial/\partial z_1, \ldots, z_j, \partial/\partial z_j, \ldots)$ and hence that governing the evolution of $f(\underline{\alpha}, t)$ is $\mathcal{L}^{\mathcal{P}} = \mathcal{L}(1 - \partial/\partial\alpha_1, \alpha_1, \ldots, 1 - \partial/\partial\alpha_j, \alpha_j, \ldots)$. Secondly, the operator analogue of $\mathcal{L}^{\mathcal{P}}$ is immediately seen to be $\mathcal{L}^{\mathcal{O}} = \mathcal{L}(1 + i\hat{p}_1, \hat{\alpha}_1, \ldots, 1 + i\hat{p}_j, \hat{\alpha}_j, \ldots)$. Finally, path-integral representations for the solution of the Fokker–Planck equations can be constructed from $\mathcal{L}^{\mathcal{F}}$ and $\mathcal{L}^{\mathcal{O}}$ and shown to be the same, if the identification

$$\alpha_i \leftrightarrow z_i^* \qquad ip_i \leftrightarrow (z_i - 1) \tag{45}$$

is made. Once the form of the path-integral has been established, coarse-graining gives a field-theoretic description of the process under consideration, allowing all the standard machinery of field theory to be used to elucidate the nature of the scaling phenomena seen in these systems.

Let us illustrate the general case by a particular example: the annihilation process $A + A \to \emptyset$. Let D be the diffusion constant of the A particles and k the reaction rate. The Liouvillian $\mathcal{L}^{\mathcal{F}}$ is easily found to be:

$$\mathcal{L}^{\mathcal{F}} = D \sum_r \sum_e \{[\pi_{r+e} a_r - \pi_r a_r] - k(\pi_r^2 - 1)a_r^2\} \tag{46}$$

where e denotes the nearest neighbour sites of r. The coarsed grained version of this Liouvillian has been studied in [13] in terms of a dynamical renormalization group approach. It turns out that this field theory is super-renormalizable; the analysis can be done in arbitrary dimension, confirming the anomalous kinetics described in the introduction.

On the other hand, one can study the problem in terms of the Poisson representation and solve the Fokker–Planck equation for $f(\underline{\alpha}, t)$ [14] or construct the corresponding field theory. The operator $\mathcal{L}^{\mathcal{O}}$ reads:

$$\mathcal{L}^{\mathcal{O}} = D \sum_r \sum_e \{[i(\hat{p}_{r+e} - \hat{p}_r)\hat{\alpha}_r] - k(2i\hat{p}_r - \hat{p}_r^2)\hat{\alpha}_r^2\} \tag{47}$$

and hence the Lagrangian of the field theory, after coarse-graining, is (cf (37)):

$$L = \int \mathrm{d}^d r \, [ip(\dot{\alpha} - D\nabla^2\alpha + 2Dk\alpha^2) - Dkp^2\alpha^2] \tag{48}$$

which is identical to the Lagrangian derived from (46) [13], once the identification discussed above is made.

We have demonstrated the relationship between the two approaches that have been used to obtain exact path-integral representations for reaction-diffusion systems directly from the master equation. Both of the methods bypass the Langevin equation since for these systems the noise is non-trivial, and it is incorrect to put additive noise in 'by hand', as some early workers did. In the Poisson representation, as originally formulated, it was not possible to investigate time-dependent phenomena, and while subsequent work did introduce time evolution into the formalism, the Fock space methods developed by Doi, and others, give a more direct access to the equal or multi-time correlation functions.

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