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Field theories and exact stochastic equations for interacting particle systems

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We consider the dynamics of interacting particles with reaction and diffusion. Starting from the underlying discrete stochastic jump process we derive a general field theory describing the dynamics of the density field, which we relate to an exact stochastic equation on the density field. We show how our field theory maps onto the original Doi-Peliti formalism, allowing us to clarify further the issue of the "imaginary" Langevin noise that appears in the context of reaction-diffusion processes. Our procedure applies to a wide class of problems and is related to large deviation functional techniques developed recently to describe fluctuations of nonequilibrium systems in the hydrodynamic limit.

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Many problems of current interest in statistical physics involve strongly interacting particles that exhibit nontrivial collective phenomena. One example is that of supercooled liquids, where the dynamics slows down dramatically as the glass transition is approached, due to the increasingly collective nature of the dynamics [1]. Other examples are given by systems of diffusing particles that branch and/or annihilate and that are subjected to an external drive; depending on the relative strength of these effects a variety of nonequilibrium transitions and anomalous scaling behavior can appear [2]. Developing theoretical techniques for such difficult problems is of great importance, in view of the diversity of situations in which they can apply, and of much broader scope than the usual equilibrium statistical mechanics. A natural framework in this context is that of field theory, which combined with perturbative renormalization group techniques has been applied successfully to a wide range of nonequilibrium phase transitions [3]. Furthermore, even in nonperturbative regimes, field theory can be very useful because it allows one to articulate different types of approximations, such as the exact renormalization group approach [4] and mode coupling theory [5,6]. A field theoretical formulation of interacting particle systems which has become somewhat standard in recent years is provided by the Doi-Peliti (DP) formalism [3]. Starting from a second-quantization representation of the master equation, one obtains, after a rather elaborate coherent state representation, a field theory in terms of two fields ϕ and $\hat{\phi}$ (see below) which has been the starting point of a very large number of studies [3]. However, besides its intrinsic complexity, the formalism appears to be fraught with difficulties. For example, the action of the field theory corresponds to a reasonable-looking Langevin equation for the density of particles, except that the noise is often complex or even purely imaginary. This suggests that the field ϕ, despite its superficial resemblance to the density, in fact lacks direct physical interpretation; see, e.g., [7,8].

The aim of this Rapid Communication is to formulate a two-field theory for interacting particles in a transparent way, starting from a natural representation of the microscopic stochastic dynamics of the system in discrete space. Our formalism focuses on the *physical* density field ρ and, as a consequence, is related directly to the stochastic equations governing the evolution of ρ. The original DP formalism is recovered by performing a canonical Cole-Hopf transformation. Our method is straightforward, free of the ambiguities related to the imaginary noise, and applies to many different situations (diffusion in an external force field, pairwise interacting particles, branching and annihilation processes, hard-core particles, etc.). Furthermore, it is related to recent techniques developed in mathematical physics (see below) [9]. As an interesting physical side product, our field theory in the case of liquids is found to be identical to the one obtained from a Martin–Siggia–Rose–De Dominicis–Janssen (MSRDJ) [10] representation of the stochastic equation on the density field derived by Dean for Langevin particles [11]. This is important since Dean's derivation contains several subtleties. In particular, some have raised concerns about a possible hidden coarse-graining procedure that would explain why the ideal gas entropy appears, quite unexpectedly, in the Langevin equation. We end the paper with various technical comments, and possible applications and extensions of our formalism.

Let us start from the simplest situation—two sites labeled 1 and 2 between which particles hop back and forth with a Poisson rate W_{12} and W_{21}. The (integer) numbers of particles on the two sites are n_1 and n_2. The variation of n_i between t and $t+dt$ will be denoted dJ_i as is standard for *Poisson jump processes* [12]; it is not a small quantity since it is equal to 0 or ± 1, but the probability for it to be nonzero is of order dt. Of course, dJ_1 and dJ_2 are strongly correlated since a particle leaving site 1 lands on site 2, and vice versa. More precisely, $dJ_1=-dJ_2=+1$ with probability $n_2 W_{21} dt$, $dJ_1=-dJ_2=-1$ with probability $n_1 W_{12} dt$, and $dJ_1=dJ_2=0$ otherwise. We now introduce, as in the MSRDJ approach, the generating function for the histories of the system: $Z(\{n,\hat{n}\})=\langle \Pi_t \exp[\hat{n}_1(t)(dJ_1-dn_1)+\hat{n}_2(t)(dJ_2-dn_2)]\rangle$, where the averaging $\langle\cdots\rangle$ is over the realizations of the Poisson jump processes. From the above rules, it is easy to find the result in the limit $dt\to 0$:

$$Z(\{n,\hat{n}\}) = \exp \int dt[-\hat{n}_1\partial_t n_1 - \hat{n}_2\partial_t n_2 + n_1 W_{12}(e^{\hat{n}_2-\hat{n}_1}-1) + n_2 W_{21}(e^{\hat{n}_1-\hat{n}_2}-1)]. \quad (1)$$

Obviously, one could add different processes, such as, for example, on-site annihilation, where $dJ_i=-1$ with probability $n_i\mu\, dt$, branching, where $dJ_i=+1$ with probability $n_i\nu\, dt$, two-body annihilation, where $dJ_i=-2$ with probability $n_i(n_i-1)\lambda\, dt$, etc. With N sites on a lattice, the total MSRDJ "action" reads $S=\ln Z$:

$$S(\{n,\hat{n}\}) = \int dt\Big(-\sum_i \hat{n}_i\partial_t n_i + \sum_{\langle ij\rangle} n_i W_{ij}(e^{\hat{n}_j-\hat{n}_i}-1) + \sum_i n_i[\mu(e^{-\hat{n}_i}-1) + \nu(e^{\hat{n}_i}-1) + \lambda(n_i-1)(e^{-2\hat{n}_i}-1)]\Big), \quad (2)$$

where $\langle ij\rangle$ means that the sum is over all couples i,j. In addition, a factorized initial condition with distribution $p(n_i(0))$ can be included by adding a contribution $\Sigma_i[-\hat{n}_i(0)n_i(0)+\ln g(\hat{n}_i(0))]$, with $g(x)=\Sigma_q p(q)e^{qx}$. As is customary in MSRDJ-type procedures [3] the average value over the stochastic dynamics of any observable O, a generic function of $\{n_i(t)\}$, equals the average of O over the field theory characterized by the action (2) and the fields $n_i,\hat{n}_i$, which should be treated as *continuous*. This ends the derivation of the field theory which, as anticipated, turns out to be much more straightforward than the DP one.

We now want to consider the continuum limit of (2). With this aim we write $W_{ij}=W_0\exp[(U_i-U_j)/2T]$ where U_i is an on-site potential (possibly time dependent), which varies on scales much larger than the lattice spacing a, and T is the temperature. Restricting consideration to nearest-neighbor hopping, we therefore write $W_{ij}=W_0(1-a\mathbf{e}_{ij}\cdot\boldsymbol{\nabla}U(\boldsymbol{x},t)/2T)$, where $\boldsymbol{x}$ is the position in space of site i and $\mathbf{e}_{ij}$ is the unit vector pointing from i to j. Defining the local density field $\rho(\boldsymbol{x},t)=n_i/a^d$ and $\hat{\rho}(\boldsymbol{x},t)=\hat{n}_i$ and expanding to second order in gradients, we finally obtain (in the $a\to 0$ limit, and with $\lambda=0$ for the time being—see below)

$$S(\{\rho,\hat{\rho}\}) = \int dt\, d\boldsymbol{x}\{-\hat{\rho}(\boldsymbol{x},t)\partial_t\rho(\boldsymbol{x},t) + \rho(\boldsymbol{x},t)[\mu(e^{-\hat{\rho}}-1) + \nu(e^{\hat{\rho}}-1)]\} - \gamma\int dt\, d\boldsymbol{x}\ \boldsymbol{\nabla}\hat{\rho}(\boldsymbol{x},t)\cdot\rho(\boldsymbol{x},t)\,\boldsymbol{\nabla}U(\boldsymbol{x},t) + \gamma T\int dt\, d\boldsymbol{x}\{-\boldsymbol{\nabla}\rho(\boldsymbol{x},t)\cdot\boldsymbol{\nabla}\hat{\rho}(\boldsymbol{x},t) + \rho(\boldsymbol{x},t)[\boldsymbol{\nabla}\hat{\rho}(\boldsymbol{x},t)]^2\}, \quad (3)$$

where $\gamma\equiv W_0a^2/2T$ is the mobility of the particles. Note that the above derivation is easily generalized to many other processes and is independent of the particular form of W_{ij} as long as detailed balance is verified (although one could also consider nonpotential force fields as well).

Before mapping this action onto the more standard DP form, we want to specialize to the case where $\mu=\nu=0$, and $U(\boldsymbol{x},t)$ comes from a two-body interaction between the particles, i.e., $U(\boldsymbol{x},t)=\int d\boldsymbol{y}\ \rho(\boldsymbol{y},t)V(\boldsymbol{x}-\boldsymbol{y})$. In this case, one finds that the above action is identical to the one obtained by using the standard MSRDJ representation for the following Langevin equation, derived by Dean for interacting Brownian particles:

$$\partial_t\rho(\boldsymbol{x},t) = \boldsymbol{\nabla}\cdot\left(\gamma\rho(\boldsymbol{x},t)\,\boldsymbol{\nabla}\frac{\partial F[\rho]}{\partial\rho} + \sqrt{\rho(\boldsymbol{x},t)}\,\boldsymbol{\eta}(\boldsymbol{x},t)\right), \quad (4)$$

where $\boldsymbol{\eta}$ is a Gaussian white noise with correlations $\langle\eta_\alpha(\boldsymbol{x},t)\eta_\beta(\boldsymbol{x}',t')\rangle=2\gamma T\delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t')$ and $F[\rho]$ is the effective free energy, which has the naively expected shape $F[\rho]=T\int d\boldsymbol{x}\ \rho(\boldsymbol{x})\ln\rho(\boldsymbol{x})+(1/2)\int d\boldsymbol{x}\,d\boldsymbol{y}\ \rho(\boldsymbol{x})V(\boldsymbol{x}-\boldsymbol{y})\rho(\boldsymbol{y})$ (note that Dean set the mobility γ of the particles to unity). This is quite remarkable, since $\rho(\boldsymbol{x},t)$ in Dean's equation is the exact continuum microscopic density of the system, $\rho(\boldsymbol{x},t)=\Sigma_i\delta(\boldsymbol{x}-\boldsymbol{r}_i(t))$, before any coarse graining [$r_i(t)$ denotes the position of particle i at time t]; it is therefore not at all trivial that the effective free energy should have a mean-field form. The fact that our derivation, which starts on a lattice and never uses Ito calculus, leads to the same action confirms the validity of Dean's analysis.

Let us now consider a Cole-Hopf change of variables from the above fields $\rho,\hat{\rho}$ to new fields $\phi,\hat{\phi}$ defined as

$$\rho(\boldsymbol{x},t) = \hat{\phi}(\boldsymbol{x},t)\phi(\boldsymbol{x},t^-) \qquad \hat{\rho}(\boldsymbol{x},t) = \ln[\hat{\phi}(\boldsymbol{x},t)]. \quad (5)$$

The Jacobian of this transformation is 1 and thus the measure is preserved. The reason for $t^-=t-\epsilon$ will be discussed in the following. Note that this change of variable could also be defined on the discrete lattice and it was already considered in the literature [3,8,13–15], but the precise connection that we establish here seems not to have been noted before. It is straightforward to show that the above action $S(\{\rho,\hat{\rho}\})$ transforms into

$$S(\{\phi,\hat{\phi}\}) = \int dt\, d\boldsymbol{x}\{\hat{\phi}[-\partial_t\phi + \gamma T\nabla^2\phi + \gamma\boldsymbol{\nabla}(\boldsymbol{\nabla}U\phi)] + (\nu-\mu\hat{\phi})\phi(1-\hat{\phi})\}. \quad (6)$$

Setting $U=0$ in the above equation, we recover exactly the DP action for the problem of diffusing, branching, and annihilating particles, usually derived in a rather thorny way from a second-quantization representation of the master equation (up to some boundary terms, which for clarity will be discussed later). Note that for $\mu=\nu=0$, the above action can be seen as the two-field representation of the propagator of the non-Hermitian Fokker-Planck operator for particles diffusing in a potential field [16]. In addition, in the case of two-body interaction between the particles, the $\boldsymbol{\nabla}(\boldsymbol{\nabla}U\phi)$ term becomes $\boldsymbol{\nabla}[\int d\boldsymbol{y}\ \phi(\boldsymbol{y},t)\hat{\phi}(\boldsymbol{y},t)\boldsymbol{\nabla}V(\boldsymbol{y}-\boldsymbol{x})\phi(\boldsymbol{x},t)]$. Let us finally remark that the mapping from the action (2) to its DP counterpart works also on the lattice; the continuum limit does not play any important role from this perspective.

The above action looks very close to a MSRDJ representation of the naive Langevin equation describing the problem

if one interprets ϕ as a density and shifts $\hat{\phi} \to \hat{\phi}+1$ in order to have $\langle \hat{\phi} \rangle = 0$ as in the usual MSRDJ method (see, e.g., [3]). However, this interpretation is problematic since, as mentioned in the introduction, the noise term is unphysical [7]. For example, in the case of diffusing particles with pairwise interaction ($\mu=\nu=0$) the "noise" term has a correlator $\langle \eta(\boldsymbol{x},t)\eta(\boldsymbol{x}',t')\rangle = 2\boldsymbol{\nabla}_x[\phi(\boldsymbol{x})(\boldsymbol{\nabla}_x V)(\boldsymbol{x}-\boldsymbol{x}')\phi(\boldsymbol{x}')]$. For a uniform density ϕ and $V(x)=V_0 \exp(-x^2)$, the variance of the noise is a negative definite operator, meaning that the noise has an imaginary part. On the other hand, we clearly see that this difficulty disappears when one uses the fields $\rho, \hat{\rho}$, which encode a very well-defined underlying Langevin equation, albeit with non-Gaussian Poisson jump terms corresponding to particle creation and annihilation.

Let us now focus on some technical but important subtleties of the transformation (5). Consider pair annihilation ($A+A \to 0$) with rate λ on a single site. The corresponding contributions in the MSRDJ and DP actions are $\lambda\rho(\rho-1)(e^{-2\hat{\rho}}-1)$ and $\lambda\phi^2(1-\hat{\phi}^2)$, which do not transform exactly into one another under (5). The underlying reason is that the two field theories correspond to different time discretizations. This makes a difference when the action contains nonlinear terms evaluated at the same position in time and space, because the response function $\langle \phi(\boldsymbol{x},t)\hat{\phi}(\boldsymbol{x},t')\rangle$ is discontinuous when $t=t'$. This can be traced back to the fact that the fields ϕ and $\hat{\phi}$ are the coherent state representations of creation and annihilation operators of the theory, a and $a^\dagger$, which satisfy $[a,a^\dagger]=1$. In the DP formalism the action is obtained after normal ordering [3] and as a consequence $\hat{\phi}(\boldsymbol{x},t)\phi(\boldsymbol{x},t)\hat{\phi}(\boldsymbol{x},t)\phi(\boldsymbol{x},t)$ is in fact the continuous time limit of $\hat{\phi}(\boldsymbol{x},t)\hat{\phi}(\boldsymbol{x},t-\epsilon)\phi(\boldsymbol{x},t-2\epsilon)\phi(\boldsymbol{x},t-3\epsilon)$. Instead, the field theory obtained from (2) through the transformation (5) has no normal ordering and therefore the term $\lambda\rho^2(\boldsymbol{x},t)$ is the continuous time limit of $\lambda\hat{\phi}(\boldsymbol{x},t)\phi(\boldsymbol{x},t-\epsilon)\hat{\phi}(\boldsymbol{x},t-2\epsilon)\phi(\boldsymbol{x},t-3\epsilon)$. Thus, to transform our field theory into the DP form, one has to use the transformation (5) and in addition to take care of the time discretization, which amounts to performing normal ordering, and to recover the -1 missing in the above example. An alternative way to make the exact connection between the two field theories is through the operator formalism. After having expressed the master equation in terms of the operators $a,a^\dagger$ one does a canonical transformation $a=e^{-\rho^\dagger}\rho$, $a^\dagger=e^{\rho^\dagger}$ such that $[\rho,\rho^\dagger]=1$. The operators $\rho,\rho^\dagger$, originally introduced in [10], lead to a different representation of the master equation. This then leads exactly, using again a coherent state representation, to the field theory that we derived above directly from the underlying stochastic process, including the correct boundary terms.

Another case where our strategy applies is that of interacting particles evolving under Newtonian dynamics, for which Doi also derived a field theory [17]. Our previous starting point consisted in deriving exact stochastic equations for the density field and then applying the MSRDJ procedure to get the field theory. For Hamiltonian dynamics, one can derive an exact deterministic equation for the density in position $\boldsymbol{r}$ and momentum $\boldsymbol{p}$ space, $\rho(\boldsymbol{x},\boldsymbol{p};t)=\Sigma_i \delta(\boldsymbol{r}-\boldsymbol{r}_i)\delta(\boldsymbol{p}-\boldsymbol{p}_i)$:

$$\partial_t \rho(\boldsymbol{x},\boldsymbol{p};t) = -\frac{1}{m}\boldsymbol{p}\cdot\partial_x \rho(\boldsymbol{x},\boldsymbol{p};t) + \int d\boldsymbol{x}'\, d\boldsymbol{p}'\, \rho(\boldsymbol{x}',\boldsymbol{p}';t)\partial_x V(\boldsymbol{x}-\boldsymbol{x}')\cdot\partial_p \rho(\boldsymbol{x},\boldsymbol{p};t). \quad (7)$$

In this case only the initial conditions are stochastic. The MSRDJ field theory corresponding to this equation maps exactly onto Doi's using the transformation, akin to (5), $\phi(\boldsymbol{x},\boldsymbol{p};t)=e^{-\hat{\rho}(\boldsymbol{x},\boldsymbol{p};t)}\rho(\boldsymbol{x},\boldsymbol{p};t)$ and $\hat{\phi}(\boldsymbol{x},\boldsymbol{p};t)=e^{\hat{\rho}(\boldsymbol{x},\boldsymbol{p};t)}$ [note that $\hat{\rho}(\boldsymbol{x},\boldsymbol{p};t)$ is the MSRDJ field conjugate to $\rho(\boldsymbol{x},\boldsymbol{p};t)$].

Finally, our formalism in the continuum limit bridges the gap between the purely microscopic Fokker-Planck evolution operator and the hydrodynamics description studied recently in the mathematical physics literature. A method to handle both the hydrodynamic limit and large and rare fluctuations around it has been developed in [9]. The starting point of this work is very close to the generating functional we used. However, in order to focus on hydrodynamic length and time scales, as done in [9], one has to consider a conjugated field $\hat{n}_i=\hat{\rho}(x/L)$ that is constrained to varying only on length scales of the order of the linear system size L. In this case the "action" or functional (2) becomes a function of the hydrodynamic density field, which represents the average density inside very large boxes, and can be related to the rate functional introduced and studied in [9]. On the other hand, the stochastic equations corresponding to our continuum limit are valid on a scale ℓ much larger than the lattice spacing a but much smaller than the system size L. As a consequence these allow one to tackle, with field theoretical techniques, dynamic phase transitions where the physically relevant length scales are much larger than a but not necessarily much larger than the (diverging) correlation length ξ. The hydrodynamic limit of [9] instead corresponds to length scales much larger than ξ.

In conclusion our procedure allows one to derive rather straightforwardly a field theory different from, but dual with, the Doi-Peliti formalism. This could be useful in cases where this by now standard framework does not work; see, e.g., [18,19]. It certainly avoids, unlike the DP approach, very cumbersome computations due to normal ordering in cases in which the rates are complicated functions of the local density. Another advantage of our approach is that it is, almost by construction, directly related to stochastic equations in the density field. The representation in terms of a stochastic equation, especially after having taken the continuum limit, is particularly appealing. It can be helpful for numerical investigations [20] since it might be more efficient to integrate numerically than to simulate the original lattice model. Furthermore, stochastic equations are very useful to encode and study universality classes as has been understood in the case of critical slowing down [21] and nonequilibrium phenomena such as surface growth [22]. Some applications of the results of this Rapid Communication are under way, for example, the study of the condensation phase transition in the zero-range process [23]. From a more general perspective our results make clear that exact stochastic equations can always be obtained, thereby avoiding phenomenological guesses which, especially for off-equilibrium cases, can be very tricky [24].

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