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# Field-theoretic Methods

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## Glossary

### **Absorbing state**

State from which, once reached, an interacting many-particle system cannot depart, not even through the aid of stochastic fluctuations.

### **Correlation function**

Quantitative measures of the correlation of random variables; usually set to vanish for statistically independent variables.

### **Critical dimension**

Borderline dimension  $d_c$  above which mean-field theory yields reliable results, while for  $d \leq d_c$  fluctuations crucially affect the system's large scale behavior.

### **External noise**

Stochastic forcing of a macroscopic system induced by random external perturbations, such as thermal noise from a coupling to a heat bath.

### **Field theory**

A representation of physical processes through continuous variables, typically governed by an exponential probability distribution.

### **Generating function**

Laplace transform of the probability distribution; all moments and correlation functions follow through appropriate partial derivatives.

### **Internal noise**

Random fluctuations in a stochastic macroscopic system originating from its internal kinetics.

### **Langevin equation**

Stochastic differential equation describing time evolution that is subject to fast random forcing.

### **Master equation**

Evolution equation for a configurational probability obtained by balancing gain and loss terms through transitions into and away from each state.

### **Mean-field approximation**

Approximative analytical approach to an interacting system with many degrees of freedom wherein spatial and temporal fluctuations as well as correlations between the constituents are neglected.

### **Order parameter**

A macroscopic density corresponding to an extensive variable that captures the symmetry and thereby characterizes the ordered state of a thermodynamic phase in thermal equilibrium. Nonequilibrium generalizations typically address appropriate stationary values in the long-time limit.

### **Perturbation expansion**

Systematic approximation scheme for an interacting and / or nonlinear system that involves a formal expansion about an exactly solvable simplification by means of a power series with respect to a small coupling.

## 1 Definition: fluctuations and correlations, field-theoretic methods

Traditionally, complex macroscopic systems are often described in terms of ordinary differential equations for the temporal evolution of the relevant (usually collective) variables. Some natural examples are particle or population densities, chemical reactant concentrations, and magnetization or polarization densities; others involve more abstract concepts such as an apt measure of activity, etc. Complex behavior often entails (diffusive) spreading, front propagation, and spontaneous or induced pattern formation. In order to capture these intriguing phenomena, a more detailed level of description is required, namely the inclusion of spatial degrees of freedom, whereupon the above quantities all become local density fields. Stochasticity, i.e., randomly occurring propagation, interactions, or reactions, frequently represents another important feature of complex systems. Such stochastic processes generate *internal noise* that may crucially affect even long-time and large-scale properties. In addition, other system variables, provided they fluctuate on time scales that are fast compared to the characteristic evolution times for the relevant quantities of interest, can be (approximately) accounted for within a Langevin description in the form of *external* additive or multiplicative noise.

A quantitative mathematical analysis of complex spatio-temporal structures and more generally cooperative behavior in stochastic interacting systems with many degrees of freedom typically relies on the study of appropriate *correlation functions*. *Field-theoretic*, i.e., spatially continuous, representations both for random processes defined through a master equation and Langevin-type stochastic differential equations have been developed since the 1970s. They provide a general framework for the computation of correlation functions, utilizing powerful tools that were originally developed in quantum many-body as well as quantum and statistical field theory. These methods allow us to construct systematic approximation schemes, e.g., *perturbative expansions* with respect to some parameter (presumed small) that measures the strength of fluctuations. They also form the basis of more sophisticated renormalization group methods which represent an especially potent device to investigate scale-invariant phenomena.

## 2 Introduction

### 2.1 Stochastic complex systems

Complex systems consist of many interacting components. As a consequence of either these interactions and / or the kinetics governing the system's temporal evolution, correlations between the constituents emerge that may induce cooperative phenomena such as (quasi-)periodic oscillations, the formation

of spatio-temporal patterns, and phase transitions between different macroscopic states. These are characterized in terms of some appropriate collective variables, often termed *order parameters*, which describe the large-scale and long-time system properties. The time evolution of complex systems typically entails random components: either, the kinetics itself follows stochastic rules (certain processes occur with given probabilities per unit time); or, we project our ignorance of various fast microscopic degrees of freedom (or our lack of interest in their detailed dynamics) into their treatment as stochastic noise.

An exact mathematical analysis of nonlinear stochastic systems with many interacting degrees of freedom is usually not feasible. One therefore has to resort to either computer simulations of corresponding stochastic cellular automata, or approximative treatments. A first step, which is widely used and often provides useful qualitative insights, consists of ignoring spatial and temporal fluctuations, and just studying equations of motion for ensemble-averaged order parameters. In order to arrive at closed equations, additional simplifications tend to be necessary, namely the factorization of correlations into powers of the mean order parameter densities. Such approximations are called *mean-field* theories; familiar examples are rate equations for chemical reaction kinetics or Landau–Ginzburg theory for phase transitions in thermal equilibrium. Yet in some situations mean-field approximations are insufficient to obtain a satisfactory quantitative description (see, e.g., the recent work collected in Refs. [1, 2]). Let us consider an illuminating example.

## 2.2 Example: Lotka–Volterra model

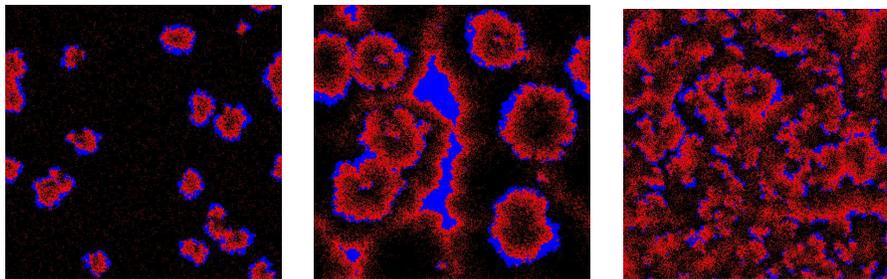
In the 1920s, Lotka and Volterra independently formulated a mathematical model to describe emerging periodic oscillations respectively in coupled autocatalytic chemical reactions, and in the Adriatic fish population (see, e.g., Murray 2002 [3]). We shall formulate the model in the language of population dynamics, and treat it as a stochastic system with two species  $A$  (the ‘predators’) and  $B$  (the ‘prey’), subject to the following reactions: predator death  $A \rightarrow \emptyset$ , with rate  $\mu$ ; prey proliferation  $B \rightarrow B + B$ , with rate  $\sigma$ ; predation interaction  $A + B \rightarrow A + A$ , with rate  $\lambda$ . Obviously, for  $\lambda = 0$  the two populations decouple; while the predators face extinction, the prey population will explode. The average predator and prey population densities  $a(t)$  and  $b(t)$  are governed by the linear differential equations  $\dot{a}(t) = -\mu a(t)$  and  $\dot{b}(t) = \sigma b(t)$ , whose solutions are exponentials. Interesting competition arises as a consequence of the nonlinear process governed by the rate  $\lambda$ . In an exact representation of the system’s temporal evolution, we would now need to know the probability of finding an  $A$ - $B$  pair at time  $t$ . Moreover, in a spatial Lotka–Volterra model, defined on a  $d$ -dimensional lattice, say, on which the individual particles can move via nearest-neighbor hopping, the predation reaction should occur only if both predators and prey occupy the same or adjacent sites. The evolution equations for the mean densities  $a(t)$  and  $b(t)$  would then have to be respectively amended by the terms  $\pm\lambda\langle a(x, t) b(x, t) \rangle$ .

Here  $a(x, t)$  and  $b(x, t)$  represent local concentrations, the brackets denote the ensemble average, and  $\langle a(x, t) b(x, t) \rangle$  represents  $A$ - $B$  cross correlations.

In the rate equation approximation, it is assumed that the local densities are uncorrelated, whereupon  $\langle a(x, t) b(x, t) \rangle$  factorizes to  $\langle a(x, t) \rangle \langle b(x, t) \rangle = a(t) b(t)$ . This yields the famous deterministic Lotka–Volterra equations

$$\dot{a}(t) = \lambda a(t) b(t) - \mu a(t) , \quad \dot{b}(t) = \sigma b(t) - \lambda a(t) b(t) . \quad (1)$$

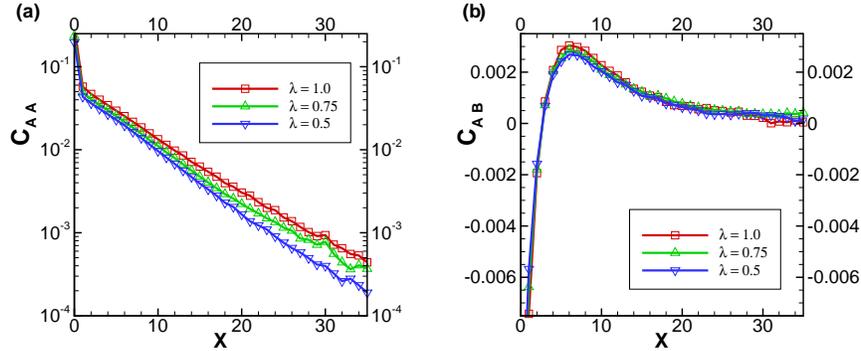
Within this mean-field approximation, the quantity  $K(t) = \lambda[a(t) + b(t)] - \sigma \ln a(t) - \mu \ln b(t)$  (essentially the system’s Lyapunov function) is a constant of motion,  $\dot{K}(t) = 0$ . This results in regular nonlinear population oscillations, whose frequency and amplitude are fully determined by the initial conditions, a rather unrealistic feature. Moreover Eqs. (1) are known to be unstable with respect to various model modifications (as discussed in Murray 2002 [3]).



**Fig. 1. Field-theoretic Methods.** Snapshots of the time evolution (left to right) of activity fronts emerging in a stochastic Lotka–Volterra model simulated on a  $512 \times 512$  lattice, with periodic boundary conditions and site occupation numbers restricted to 0 or 1. For the chosen reaction rates, the system is in the species coexistence phase (with rates  $\sigma = 4.0$ ,  $\mu = 0.1$ , and  $\lambda = 2.2$ ), and the corresponding mean-field fixed point a focus. The red, blue, and black dots respectively represent predators  $A$ , prey  $B$ , and empty sites  $\emptyset$ . Reproduced with permission from Ref. [4].

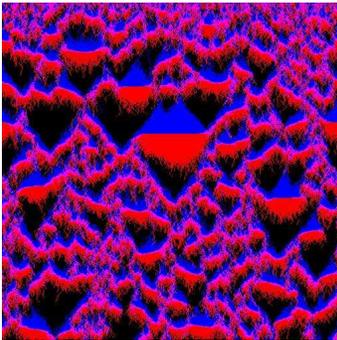
In contrast with the rate equation predictions, the original stochastic spatial Lotka–Volterra system displays much richer behavior (a recent overview is presented in Ref. [4]): The predator–prey coexistence phase is governed, for sufficiently large values of the predation rate, by an incessant sequence of ‘pursuit and evasion’ wave fronts that form quite complex dynamical patterns, as depicted in Figure 1, which shows snapshots taken in a two-dimensional lattice Monte Carlo simulation where each site could at most be occupied by a single particle. In finite systems, these correlated structures induce erratic population oscillations whose features are independent of the initial configuration. Moreover, if locally the prey ‘carrying capacity’ is limited (corresponding to restricting the maximum site occupation number per lattice site), there appears an extinction threshold for the predator population that separates the active coexistence regime through a continuous phase transition from a state

wherein at long times  $t \rightarrow \infty$  only prey survive. With respect to the predator population, this represents an *absorbing state*: once all  $A$  particles have vanished, they cannot be produced by the stochastic kinetics.



**Fig. 2. Field-theoretic Methods.** Static correlation functions (a)  $C_{AA}(x)$  (note the logarithmic scale), and (b)  $C_{AB}(x)$ , measured in simulations on a  $1024 \times 1024$  lattice without any restrictions on the site occupations. The reaction rates were  $\sigma = 0.1$ ,  $\mu = 0.1$ , and  $\lambda$  was varied from 0.5 (blue triangles, upside down), 0.75 (green triangles), to 1.0 (red squares). Reproduced with permission from Ref. [5].

A quantitative characterization of the emerging spatial structures utilizes equal-time correlation functions such as  $C_{AA}(x - x', t) = \langle a(x, t) a(x', t) \rangle - a(t)^2$  and  $C_{AB}(x - x', t) = \langle a(x, t) b(x', t) \rangle - a(t) b(t)$ , computed at some large time  $t$  in the (quasi-)stationary state. These are shown in Figure 2 as measured in computer simulations for a stochastic Lotka–Volterra model (but here no restrictions on the site occupation numbers of the  $A$  or  $B$  particles were implemented). The  $A$ - $A$  (and  $B$ - $B$ ) correlations obviously decay essentially exponentially with distance  $x$ ,  $C_{AA}(x) \propto C_{BB}(x) \propto e^{-|x|/\xi}$ , with roughly equal correlation lengths  $\xi$  for the predators and prey. The cross-correlation function  $C_{AB}(x)$  displays a maximum at six lattice spacings; these positive correlations indicate the spatial extent of the emerging activity fronts (prey followed by the predators). At closer distance, the  $A$  and  $B$  particles become *anti-correlated* ( $C_{AB}(x) < 0$  for  $|x| < 3$ ): prey would not survive close encounters with the predators. In a similar manner, one can address temporal correlations. These appear prominently in the space-time plot of Figure 3 obtained for a Monte Carlo run on a one-dimensional lattice (no site occupation restrictions), indicating localized population explosion and extinction events.



**Fig. 3. Field-theoretic Methods.** Space-time plot (space horizontal, with periodic boundary conditions; time vertical, proceeding downward) showing the temporal evolution of a one-dimensional stochastic Lotka–Volterra model on 512 lattice sites, but without any restrictions on the site occupation numbers (red: predators, blue: prey, magenta: sites occupied by both species; rates:  $\sigma = 0.1$ ,  $\mu = 0.1$ ,  $\lambda = 0.1$ ). Reproduced with permission from Ref. [5].

### 3 Correlation functions and field theory

The above example demonstrates that stochastic fluctuations and correlations induced by the dynamical interactions may lead to important features that are not adequately described by mean-field approaches. We thus require tools that allow us to systematically account for fluctuations in the mathematical description of stochastic complex systems and evaluate characteristic correlations. Such a toolbox is provided through *field theory* representations that are conducive to the identification of underlying symmetries and have proven useful starting points for the construction of various approximation schemes. These methods were originally devised and elaborated in the theory of (quantum and classical) many-particle systems and quantum fields (Refs. [6]–[13] represent a sample of recent textbooks).

#### 3.1 Generating functions

The basic structure of these field theories rests in a (normalized) exponential probability distribution  $\mathcal{P}[S_i]$  for the  $N$  relevant variables  $S_i$ ,  $i = 1, \dots, N$ :  $\int \prod_{i=1}^N dS_i \mathcal{P}[S_i] = 1$ , where the integration extends over the allowed range of values for the  $S_i$ ; i.e.,

$$\mathcal{P}[S_i] = \frac{1}{\mathcal{Z}} \exp(-\mathcal{A}[S_i]) , \quad \mathcal{Z} = \int \prod_{i=1}^N dS_i \exp(-\mathcal{A}[S_i]) . \quad (2)$$

In canonical equilibrium statistical mechanics,  $\mathcal{A}[S_i] = \mathcal{H}[S_i]/k_B T$  is essentially the Hamiltonian, and the normalization is the partition function  $\mathcal{Z}$ . In Euclidean quantum field theory, the action  $\mathcal{A}[S_i]$  is given by the Lagrangian.

All observables  $\mathcal{O}$  should be functions of the basic degrees of freedom  $S_i$ ; their ensemble average thus becomes

$$\langle \mathcal{O}[S_i] \rangle = \int \prod_{i=1}^N dS_i \mathcal{O}[S_i] \mathcal{P}[S_i] = \frac{1}{\mathcal{Z}} \int \prod_{i=1}^N dS_i \mathcal{O}[S_i] \exp(-\mathcal{A}[S_i]) . \quad (3)$$

If we are interested in  $n$ -point correlations, i.e., expectation values of the products of the variables  $S_i$ , it is useful to define a *generating function*

$$\mathcal{W}[j_i] = \left\langle \exp \sum_{i=1}^N j_i S_i \right\rangle , \quad (4)$$

with  $\mathcal{W}[j_i = 0] = 1$ . Notice that  $\mathcal{W}[j_i]$  formally is just the Laplace transform of the probability distribution  $\mathcal{P}[S_i]$ . The correlation functions can now be obtained via partial derivatives of  $\mathcal{W}[j_i]$  with respect to the sources  $j_i$ :

$$\langle S_{i_1} \dots S_{i_n} \rangle = \frac{\partial}{\partial j_{i_1}} \dots \frac{\partial}{\partial j_{i_n}} \mathcal{W}[j_i] \Big|_{j_i=0} . \quad (5)$$

Connected correlation functions or cumulants can be found by similar partial derivatives of the logarithm of the generating function:

$$\langle S_{i_1} \dots S_{i_n} \rangle_c = \frac{\partial}{\partial j_{i_1}} \dots \frac{\partial}{\partial j_{i_n}} \ln \mathcal{W}[j_i] \Big|_{j_i=0} , \quad (6)$$

e.g.,  $\langle S_i \rangle_c = \langle S_i \rangle$ , and  $\langle S_i S_j \rangle_c = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle = \langle (S_i - \langle S_i \rangle) (S_j - \langle S_j \rangle) \rangle$ .

### 3.2 Perturbation expansion

For a Gaussian action, i.e., a quadratic form  $\mathcal{A}_0[S_i] = \frac{1}{2} \sum_{i,j} S_i A_{ij} S_j$  (for simplicity we assume real variables  $S_i$ ), one may readily compute the corresponding generating function  $\mathcal{W}_0[j_i]$ . After diagonalizing the symmetric  $N \times N$  matrix  $A_{ij}$ , completing the squares, and evaluating the ensuing Gaussian integrals, one obtains

$$\mathcal{Z}_0 = \frac{(2\pi)^{N/2}}{\sqrt{\det A}} , \quad \mathcal{W}_0[j_i] = \exp\left(\frac{1}{2} \sum_{i,j=1}^N j_i A_{ij}^{-1} j_j\right), \quad \langle S_i S_j \rangle_0 = A_{ij}^{-1} . \quad (7)$$

Thus, the two-point correlation functions in the Gaussian ensemble are given by the elements of the inverse harmonic coupling matrix. An important special property of the Gaussian ensemble is that all  $n$ -point functions with odd  $n$  vanish, whereas those with even  $n$  factorize into sums of all possible permutations of products of two-point functions  $A_{ij}^{-1}$  that can be constructed by pairing up the variables  $S_i$  (Wick's theorem). For example, the four-point function reads  $\langle S_i S_j S_k S_l \rangle_0 = A_{ij}^{-1} A_{kl}^{-1} + A_{ik}^{-1} A_{jl}^{-1} + A_{il}^{-1} A_{jk}^{-1}$ .

Let us now consider a general action, isolate the Gaussian contribution, and label the remainder as the nonlinear, anharmonic, or interacting part,  $\mathcal{A}[S_i] = \mathcal{A}_0[S_i] + \mathcal{A}_{\text{int}}[S_i]$ . We then observe that

$$\mathcal{Z} = \mathcal{Z}_0 \left\langle \exp\left(-\mathcal{A}_{\text{int}}[S_i]\right) \right\rangle_0, \quad \langle \mathcal{O}[S_i] \rangle = \frac{\left\langle \mathcal{O}[S_i] \exp\left(-\mathcal{A}_{\text{int}}[S_i]\right) \right\rangle_0}{\left\langle \exp\left(-\mathcal{A}_{\text{int}}[S_i]\right) \right\rangle_0}, \quad (8)$$

where the index 0 indicates that the expectation values are computed in the Gaussian ensemble. The nonlinear terms in Eq. (8) may now be treated perturbatively by expanding the exponentials in the numerator and denominator with respect to the interacting part  $\mathcal{A}_{\text{int}}[S_i]$ :

$$\langle \mathcal{O}[S_i] \rangle = \frac{\left\langle \mathcal{O}[S_i] \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left(-\mathcal{A}_{\text{int}}[S_i]\right)^{\ell} \right\rangle_0}{\left\langle \sum_{\ell=0}^{\infty} \frac{1}{\ell!} \left(-\mathcal{A}_{\text{int}}[S_i]\right)^{\ell} \right\rangle_0}. \quad (9)$$

If the interaction terms are polynomial in the variables  $S_i$ , Wick's theorem reduces the calculation of  $n$ -point functions to a summation of products of Gaussian two-point functions. Since the number of contributing terms grows factorially with the order  $\ell$  of the perturbation expansion, graphical representations in terms of Feynman diagrams become very useful for the classification and evaluation of the different contributions to the perturbation series. Basically, they consist of lines representing the Gaussian two-point functions ('propagators') that are connected to vertices that stem from the (polynomial) interaction terms; for details, see, e.g., Refs. [6]–[13].

### 3.3 Continuum limit and functional integrals

Discrete spatial degrees of freedom are already contained in the above formal description: for example, on a  $d$ -dimensional lattice with  $N_d$  sites the index  $i$  for the fields  $S_i$  merely needs to entail the site labels, and the total number of degrees of freedom is just  $N = N_d$  times the number of independent relevant quantities. Upon discretizing time, these prescriptions can be extended in effectively an additional dimension to systems with temporal evolution. We may at last take the *continuum limit* by letting  $N \rightarrow \infty$ , while the lattice constant and elementary time step tend to zero in such a manner that macroscopic dynamical features are preserved. Formally, this replaces sums over lattice sites and time steps with spatial and temporal integrations; the action  $\mathcal{A}[S_i]$  becomes a functional of the fields  $S_i(x, t)$ ; partial derivatives turn into functional derivatives; and functional integrations  $\int \prod_{i=1}^N dS_i \rightarrow \int \mathcal{D}[S_i]$  are to be inserted in the previous expressions. For example, Eqs. (3), (4), and (6) become

$$\langle \mathcal{O}[S_i] \rangle = \frac{1}{\mathcal{Z}} \int \mathcal{D}[S_i] \mathcal{O}[S_i] \exp\left(-\mathcal{A}[S_i]\right), \quad (10)$$

$$\mathcal{W}[j_i] = \left\langle \exp \int d^d x \int dt \sum_i j_i(x, t) S_i(x, t) \right\rangle, \quad (11)$$

$$\left\langle \prod_{j=1}^n S_{i_j}(x_j, t_j) \right\rangle_c = \prod_{j=1}^n \frac{\delta}{\delta j_{i_j}(x_j, t_j)} \ln \mathcal{W}[j_i] \Big|_{j_i=0}. \quad (12)$$

Thus we have arrived at a continuum field theory. Nevertheless, we may follow the procedures outlined above; specifically, the perturbation expansion expressions (8) and (9) still hold, yet with arguments  $S_i(x, t)$  that are now fields depending on continuous space-time parameters.

More than thirty years ago, Janssen and De Dominicis independently derived a mapping of the stochastic kinetics defined through nonlinear Langevin equations onto a field theory action (Janssen 1976 [14], De Dominicis 1976 [15]; reviewed in Janssen 1979 [16]). Almost simultaneously, Doi constructed a Fock space representation and therefrom a stochastic field theory for classical interacting particle systems from the master equation describing the corresponding stochastic processes (Doi 1976 [17, 18]). His approach was further developed by several authors into a powerful method for the study of internal noise and correlation effects in reaction-diffusion systems (Grassberger and Scheunert 1980 [19], Peliti 1985 [20], Peliti 1986 [21], Lee 1995 [22], Lee and Cardy 1995 [23]; for recent reviews, see Refs. [24, 25]). We shall see below that the field-theoretic representations of both classical master and Langevin equations require *two* independent fields for each stochastic variable. Otherwise, the computation of correlation functions and the construction of perturbative expansions fundamentally works precisely as sketched above. But the underlying causal temporal structure induces important specific features such as the absence of ‘vacuum diagrams’ (closed response loops): the denominator in Eq. (2) is simply  $\mathcal{Z} = 1$ . (For unified and more detailed descriptions of both versions of dynamic stochastic field theories, see Refs. [26, 27].)

## 4 Discrete stochastic interacting particle systems

We first outline the mapping of stochastic interacting particle dynamics as defined through a master equation onto a field theory action [17]–[23]. Let us denote the configurational probability for a stochastically evolving system to be in state  $\alpha$  at time  $t$  with  $P(\alpha; t)$ . Given the transition rates  $W_{\alpha \rightarrow \beta}(t)$  from states  $\alpha$  to  $\beta$ , a *master equation* essentially balances the transitions into and out of each state:

$$\frac{\partial P(\alpha; t)}{\partial t} = \sum_{\beta \neq \alpha} \left[ W_{\beta \rightarrow \alpha}(t) P(\beta; t) - W_{\alpha \rightarrow \beta}(t) P(\alpha; t) \right]. \quad (13)$$

The dynamics of many complex systems can be cast into the language of ‘chemical’ reactions, wherein certain particle species (upon encounter, say) transform into different species with fixed (time-independent) reaction rates.

The ‘particles’ considered here could be atoms or molecules in chemistry, but also individuals in population dynamics (as in our example in section 2.2), or appropriate effective degrees of freedom governing the system’s kinetics, such as domain walls in magnets, etc. To be specific, we envision our particles to propagate via unbiased random walks (diffusion) on a  $d$ -dimensional hypercubic lattice, with the reactions occurring according to prescribed rules when particles meet on a lattice site. This stochastic interacting particle system is then at any time fully characterized by the number of particles  $n_A, n_B, \dots$  of each species  $A, B, \dots$  located on any lattice site. The following describes the construction of an associated field theory action. As important examples, we briefly discuss annihilation reactions and absorbing state phase transitions.

#### 4.1 Master equation and Fock space representation

The formal procedures are best explained by means of a simple example; thus consider the irreversible binary annihilation process  $A + A \rightarrow A$ , happening with rate  $\lambda$ . In terms of the occupation numbers  $n_i$  of the lattice sites  $i$ , we can construct the master equation associated with these on-site reactions as follows. The annihilation process locally changes the occupation numbers by one; the transition rate from a state with  $n_i$  particles at site  $i$  to  $n_i - 1$  particles is  $W_{n_i \rightarrow n_i - 1} = \lambda n_i (n_i - 1)$ , whence

$$\frac{\partial P(n_i; t)}{\partial t} = \lambda (n_i + 1) n_i P(n_i + 1; t) - \lambda n_i (n_i - 1) P(n_i; t) \quad (14)$$

represents the master equation for this reaction at site  $i$ . As an initial condition, we can for example choose a Poisson distribution  $P(n_i) = \bar{n}_0^{n_i} e^{-\bar{n}_0} / n_i!$  with mean initial particle density  $\bar{n}_0$ . In order to capture the complete stochastic dynamics, we just need to add similar contributions describing other processes, and finally sum over all lattice sites  $i$ .

Since the reactions all change the site occupation numbers by integer values, a Fock space representation (borrowed from quantum mechanics) turns out particularly useful. To this end, we introduce the harmonic oscillator or bosonic ladder operator algebra  $[a_i, a_j] = 0 = [a_i^\dagger, a_j^\dagger]$ ,  $[a_i, a_j^\dagger] = \delta_{ij}$ , from which we construct the particle number eigenstates  $|n_i\rangle$ , namely  $a_i |n_i\rangle = n_i |n_i - 1\rangle$ ,  $a_i^\dagger |n_i\rangle = |n_i + 1\rangle$ ,  $a_i^\dagger a_i |n_i\rangle = n_i |n_i\rangle$ . (Notice that a different normalization than in ordinary quantum mechanics has been employed here.) A general state with  $n_i$  particles on sites  $i$  is obtained from the ‘vacuum’ configuration  $|0\rangle$ , defined via  $a_i |0\rangle = 0$ , through the product  $|\{n_i\}\rangle = \prod_i a_i^{\dagger n_i} |0\rangle$ .

To implement the stochastic kinetics, we introduce a formal state vector as a linear combination of all possible states weighted by the time-dependent configurational probability:

$$|\Phi(t)\rangle = \sum_{\{n_i\}} P(\{n_i\}; t) |\{n_i\}\rangle. \quad (15)$$

Simple manipulations then transform the linear time evolution according to the master equation into an ‘imaginary-time’ Schrödinger equation

$$\frac{\partial |\Phi(t)\rangle}{\partial t} = -H |\Phi(t)\rangle, \quad |\Phi(t)\rangle = e^{-Ht} |\Phi(0)\rangle \quad (16)$$

governed by a stochastic quasi-Hamiltonian (rather, the Liouville time evolution operator). For on-site reaction processes,  $H_{\text{reac}} = \sum_i H_i(a_i^\dagger, a_i)$  is a sum of local contributions; e.g., for the binary annihilation reaction,  $H_i(a_i^\dagger, a_i) = -\lambda(1-a_i^\dagger) a_i^\dagger a_i^2$ . It is a straightforward exercise to construct the corresponding expressions within this formalism for the generalization  $kA \rightarrow \ell A$ ,

$$H_i(a_i^\dagger, a_i) = -\lambda \left( a_i^{\dagger\ell} - a_i^{\dagger k} \right) a_i^k, \quad (17)$$

and for nearest-neighbor hopping with rate  $D$  between adjacent sites  $\langle ij \rangle$ ,

$$H_{\text{diff}} = D \sum_{\langle ij \rangle} \left( a_i^\dagger - a_j^\dagger \right) \left( a_i - a_j \right). \quad (18)$$

The two contributions for each process may be interpreted as follows: The first term in Eq. (17) corresponds to the actual process, and describes how many particles are annihilated and (re-)created in each reaction. The second term encodes the ‘order’ of each reaction, i.e., the number operator  $a_i^\dagger a_i$  appears to the  $k$ th power, but in the normal-ordered form  $a_i^{\dagger k} a_i^k$ , for a  $k$ th-order process. These procedures are readily adjusted for reactions involving multiple particle species. We merely need to specify the occupation numbers on each site and correspondingly introduce additional ladder operators  $b_i, c_i, \dots$  for each new species, with  $[a_i, b_i^\dagger] = 0 = [a_i, c_i^\dagger]$  etc. For example, consider the reversible reaction  $kA + \ell B \rightleftharpoons mC$  with forward rate  $\lambda$  and backward rate  $\sigma$ ; the associated reaction Hamiltonian reads

$$H_{\text{reac}} = - \sum_i \left( c_i^{\dagger m} - a_i^{\dagger k} b_i^{\dagger \ell} \right) \left( \lambda a_i^k b_i^\ell - \sigma c_i^m \right). \quad (19)$$

Similarly, for the Lotka–Volterra model of section 2.2, one finds

$$H_{\text{reac}} = - \sum_i \left[ \mu \left( 1 - a_i^\dagger \right) a_i + \sigma \left( b_i^\dagger - 1 \right) b_i^\dagger b_i + \lambda \left( a_i^\dagger - b_i^\dagger \right) a_i^\dagger a_i b_i \right]. \quad (20)$$

Note that all the above quasi-Hamiltonians are non-Hermitian operators, which naturally reflects the creation and destruction of particles.

Our goal is to compute averages and correlation functions with respect to the configurational probability  $P(\{n_i\}; t)$ . Returning to a single-species system (again, the generalization to many particle species is obvious), this is accomplished with the aid of the projection state  $\langle \mathcal{P} | = \langle 0 | \prod_i e^{a_i}$ , for which  $\langle \mathcal{P} | 0 \rangle = 1$  and  $\langle \mathcal{P} | a_i^\dagger = \langle \mathcal{P} |$ , since  $[e^{a_i}, a_j^\dagger] = e^{a_i} \delta_{ij}$ . For the desired statistical

averages of observables (which must all be expressible as functions of the occupation numbers  $\{n_i\}$ ), one obtains

$$\langle \mathcal{O}(t) \rangle = \sum_{\{n_i\}} \mathcal{O}(\{n_i\}) P(\{n_i\}; t) = \langle \mathcal{P} | \mathcal{O}(\{a_i^\dagger a_i\}) | \Phi(t) \rangle . \quad (21)$$

For example, as a consequence of probability conservation,  $1 = \langle \mathcal{P} | \Phi(t) \rangle = \langle \mathcal{P} | e^{-Ht} | \Phi(0) \rangle$ . Thus necessarily  $\langle \mathcal{P} | H = 0$ ; upon commuting  $e^{\sum_i a_i}$  with  $H$ , the creation operators are shifted  $a_i^\dagger \rightarrow 1 + a_i^\dagger$ , whence this condition is fulfilled provided  $H_i(a_i^\dagger \rightarrow 1, a_i) = 0$ , which is indeed satisfied by our above explicit expressions (17) and (18). Through this prescription, we may replace  $a_i^\dagger a_i \rightarrow a_i$  in all averages; e.g., the particle density becomes  $a(t) = \langle a_i(t) \rangle$ .

In the bosonic operator representation above, we have assumed that no restrictions apply to the particle occupation numbers  $n_i$  on each site. If  $n_i \leq 2s + 1$ , one may instead employ a representation in terms of spin  $s$  operators. For example, particle exclusion systems with  $n_i = 0$  or 1 can thus be mapped onto non-Hermitian spin 1/2 ‘quantum’ systems (for recent overviews, see Refs. [28, 29]). Specifically in one dimension, such representations in terms of integrable spin chains have been very fruitful. An alternative approach uses the bosonic theory, but incorporates the site occupation restrictions through exponentials in the number operators  $e^{-a_i^\dagger a_i}$  (van Wijland 2001 [30]).

## 4.2 Continuum limit and field theory

As a next step, we follow an established route in quantum many-particle theory [8] and proceed towards a field theory representation through constructing the path integral equivalent to the ‘Schrödinger’ dynamics (16) based on coherent states, which are right eigenstates of the annihilation operator,  $a_i |\phi_i\rangle = \phi_i |\phi_i\rangle$ , with complex eigenvalues  $\phi_i$ . Explicitly,  $|\phi_i\rangle = \exp\left(-\frac{1}{2} |\phi_i|^2 + \phi_i a_i^\dagger\right) |0\rangle$ , and these coherent states satisfy the overlap formula  $\langle \phi_j | \phi_i \rangle = \exp\left(-\frac{1}{2} |\phi_i|^2 - \frac{1}{2} |\phi_j|^2 + \phi_j^* \phi_i\right)$ , and the (over-)completeness relation  $\int \prod_i d^2 \phi_i |\{\phi_i\}\rangle \langle \{\phi_i\}| = \pi$ . Upon splitting the temporal evolution (16) into infinitesimal increments, standard procedures (elaborated in detail in Ref. [25]) eventually yield an expression for the configurational average

$$\langle \mathcal{O}(t) \rangle \propto \int \prod_i d\phi_i d\phi_i^* \mathcal{O}(\{\phi_i\}) e^{-\mathcal{A}[\phi_i^*, \phi_i; t]} , \quad (22)$$

which is of the form (3), with the action

$$\mathcal{A}[\phi_i^*, \phi_i; t_f] = \sum_i \left( -\phi_i(t_f) + \int_0^{t_f} dt \left[ \phi_i^* \frac{\partial \phi_i}{\partial t} + H_i(\phi_i^*, \phi_i) \right] - \bar{n}_0 \phi_i^*(0) \right) , \quad (23)$$

where the first term originates from the projection state, and the last one stems from the initial Poisson distribution. Through this procedure, in the

original quasi-Hamiltonian the creation and annihilation operators  $a_i^\dagger$  and  $a_i$  are simply replaced with the complex numbers  $\phi_i^*$  and  $\phi_i$ .

Finally, we proceed to the continuum limit,  $\phi_i(t) \rightarrow \psi(\mathbf{x}, t)$ ,  $\phi_i^*(t) \rightarrow \hat{\psi}(\mathbf{x}, t)$ . The ‘bulk’ part of the action then becomes

$$\mathcal{A}[\hat{\psi}, \psi] = \int d^d x \int dt \left[ \hat{\psi} \left( \frac{\partial}{\partial t} - D \nabla^2 \right) \psi + \mathcal{H}_{\text{reac}}(\hat{\psi}, \psi) \right], \quad (24)$$

where the discrete hopping contribution (18) has naturally turned into a continuum diffusion term. We have thus arrived at a *microscopic* field theory for stochastic reaction–diffusion processes, without invoking any assumptions on the form or correlations of the internal reaction noise. Note that we require two independent fields  $\hat{\psi}$  and  $\psi$  to capture the stochastic dynamics. Actions of the type (24) may serve as a basis for further systematic coarse-graining, constructing a perturbation expansion as outlined in section 3.2, and perhaps a subsequent renormalization group analysis [25]–[27]. We remark that it is often useful to perform a shift in the field  $\hat{\psi}$  about the mean-field solution,  $\hat{\psi}(x, t) = 1 + \tilde{\psi}(x, t)$ . For occasionally, the resulting field theory action allows the derivation of an equivalent Langevin dynamics, see section 5 below.

### 4.3 Annihilation processes

Let us consider our simple single-species example  $kA \rightarrow \ell A$ . The reaction part of the corresponding field theory action reads

$$\mathcal{H}_{\text{reac}}(\hat{\psi}, \psi) = -\lambda \left( \hat{\psi}^\ell - \hat{\psi}^k \right) \psi^k, \quad (25)$$

see Eq. (17). It is instructive to study the *classical field equations*, namely  $\delta\mathcal{A}/\delta\psi = 0$ , which is always solved by  $\hat{\psi} = 1$ , reflecting probability conservation, and  $\delta\mathcal{A}/\delta\hat{\psi} = 0$ , which, upon inserting  $\hat{\psi} = 1$  yields

$$\frac{\partial\psi(x, t)}{\partial t} = D \nabla^2 \psi(x, t) - (k - \ell) \lambda \psi(x, t)^k, \quad (26)$$

i.e., the mean-field equation for the local particle density  $\psi(x, t)$ , supplemented with a diffusion term. For  $k = 1$ , the particle density grows ( $k < \ell$ ) or decays ( $k > \ell$ ) exponentially. The solution of the rate equation for  $k > 1$ ,  $a(t) = \langle \psi(x, t) \rangle = [a(0)^{1-k} + (k - \ell)(k - 1) \lambda t]^{-1/(k-1)}$  implies a divergence within a finite time for  $k < \ell$ , and an algebraic decay  $\sim (\lambda t)^{-1/(k-1)}$  for  $k > \ell$ .

The full field theory action, which was derived from the master equation defining the very stochastic process, provides a means of systematically including fluctuations in the mathematical treatment. Through a dimensional analysis, we can determine the (upper) *critical dimension* below which fluctuations become sufficiently strong to alter these power laws. Introducing an inverse length scale  $\kappa$ ,  $[x] \sim \kappa^{-1}$ , and applying diffusive temporal scaling,  $[D t] \sim \kappa^{-2}$ ,

and  $[\hat{\psi}(x, t)] \sim \kappa^0$ ,  $[\psi(x, t)] \sim \kappa^d$  in  $d$  spatial dimensions, the reaction rate in terms of the diffusivity scales according to  $[\lambda/D] \sim \kappa^{2-(k-1)d}$ . In large dimensions, the kinetics is *reaction-limited*, and at least qualitatively correctly described by the mean-field rate equation. In low dimensions, the dynamics becomes *diffusion-limited*, and the annihilation reactions generate depletion zones and spatial particle anti-correlations that slow down the density decay. The nonlinear coupling  $\lambda/D$  becomes dimensionless at the boundary critical dimension  $d_c(k) = 2/(k-1)$  that separates these two distinct regimes. Thus in physical dimensions, intrinsic stochastic fluctuations are relevant only for pair and triplet annihilation reactions. By means of a renormalization group analysis (for details, see Ref. [25]) one finds for  $k = 2$  and  $d < d_c(2) = 2$ :  $a(t) \sim (Dt)^{-d/2}$  [21, 22], as confirmed by exact solutions in one dimension. Precisely at the critical dimension, the mean-field decay laws acquire logarithmic corrections, namely  $a(t) \sim (Dt)^{-1} \ln(Dt)$  for  $k = 2$  at  $d_c(2) = 2$ , and  $a(t) \sim [(Dt)^{-1} \ln(Dt)]^{1/2}$  for  $k = 3$  at  $d_c(3) = 1$ . Annihilation reaction between different species (e.g.,  $A + B \rightarrow \emptyset$ ) may introduce additional correlation effects, such as particle segregation and the confinement of active dynamics to narrow reaction zones [23]; a recent overview can be found in Ref. [25].

#### 4.4 Active to absorbing state phase transitions

Competition between particle production and decay processes leads to even richer scenarios, and can induce genuine nonequilibrium transitions that separate ‘active’ phases (wherein the particle densities remain nonzero in the long-time limit) from ‘inactive’ stationary states (where the concentrations ultimately vanish). A special but abundant case are *absorbing states*, where, owing to the absence of any agents, stochastic fluctuations cease entirely, and no particles can be regenerated [31, 32]. These occur in a variety of systems in nature (Refs. [33, 34] contain extensive discussions of various model systems); examples are chemical reactions involving an inert state  $\emptyset$ , wherefrom no reactants  $A$  are released anymore, or stochastic population dynamics models, combining diffusive migration of a species  $A$  with asexual reproduction  $A \rightarrow 2A$  (with rate  $\sigma$ ), spontaneous death  $A \rightarrow \emptyset$  (at rate  $\mu$ ), and lethal competition  $2A \rightarrow A$  (with rate  $\lambda$ ). In the inactive state, where no population members  $A$  are left, clearly all processes terminate. Similar effective dynamics may be used to model certain nonequilibrium physical systems, such as the domain wall kinetics in Ising chains with competing Glauber and Kawasaki dynamics. Here, spin flips  $\uparrow\uparrow\downarrow \rightarrow \uparrow\uparrow\uparrow$  and  $\uparrow\uparrow\downarrow \rightarrow \uparrow\uparrow\uparrow$  may be viewed as domain wall ( $A$ ) hopping and pair annihilation  $2A \rightarrow \emptyset$ , whereas spin exchange  $\uparrow\uparrow\downarrow \rightarrow \uparrow\downarrow\uparrow$  represents a branching process  $A \rightarrow 3A$ . Notice that the para- and ferromagnetic phases respectively map onto the active and inactive ‘particle’ states. The ferromagnetic state becomes absorbing if the spin flip rates are taken at zero temperature.

The reaction quasi-Hamiltonian corresponding to the stochastic dynamics of the aforementioned population dynamics model reads

$$\mathcal{H}_{\text{reac}}(\hat{\psi}, \psi) = (1 - \hat{\psi}) (\sigma \hat{\psi} \psi - \mu \psi - \lambda \hat{\psi} \psi^2) . \quad (27)$$

The associated rate equation is the Fisher–Kolmogorov equation (see Murray 2002 [3])

$$\dot{a}(t) = (\sigma - \mu) a(t) - \lambda a(t)^2 , \quad (28)$$

which yields both inactive and active phases: For  $\sigma < \mu$  we have  $a(t \rightarrow \infty) \rightarrow 0$ , whereas for  $\sigma > \mu$  the density eventually saturates at  $a_s = (\sigma - \mu)/\lambda$ . The explicit time-dependent solution  $a(t) = a(0) a_s / [a(0) + [a_s - a(0)] e^{(\mu - \sigma)t}]$  shows that both stationary states are approached exponentially in time. They are separated by a continuous nonequilibrium phase transition at  $\sigma = \mu$ , where the temporal decay becomes algebraic,  $a(t) = a(0)/[1 + a(0)\lambda t] \rightarrow 1/(\lambda t)$  as  $t \rightarrow \infty$ , independent of the initial density  $a(0)$ . As in second-order equilibrium phase transitions, however, critical fluctuations are expected to invalidate the mean-field power laws in low dimensions  $d < d_c$ .

If we now shift the field  $\hat{\psi}$  about its stationary value 1 and rescale according to  $\hat{\psi}(\mathbf{x}, t) = 1 + \sqrt{\sigma/\lambda} \tilde{S}(\mathbf{x}, t)$  and  $\psi(\mathbf{x}, t) = \sqrt{\lambda/\sigma} S(\mathbf{x}, t)$ , the (bulk) action becomes

$$\mathcal{A}[\tilde{S}, S] = \int d^d x \int dt \left[ \tilde{S} \left( \frac{\partial}{\partial t} + D(r - \nabla^2) \right) S - u (\tilde{S} - S) \tilde{S} S + \lambda \tilde{S}^2 S^2 \right] . \quad (29)$$

Thus, the three-point vertices have been scaled to identical coupling strengths  $u = \sqrt{\sigma \lambda}$ , which in fact represents the effective coupling of the perturbation expansion. Its scaling dimension is  $[u] = \mu^{2-d/2}$ , whence we infer the upper critical dimension  $d_c = 4$ . The four-point vertex  $\propto \lambda$ , with  $[\lambda] = \mu^{2-d}$ , is then found to be irrelevant in the renormalization group sense, and can be dropped for the computation of universal, asymptotic scaling properties. The action (29) with  $\lambda = 0$  is known as Reggeon field theory (Moshe 1978 [35]); it satisfies a characteristic symmetry, namely invariance under so-called rapidity inversion  $S(\mathbf{x}, t) \leftrightarrow -\tilde{S}(\mathbf{x}, -t)$ . Remarkably, it has moreover been established that the field theory action (29) describes the scaling properties of critical directed percolation clusters [36]–[38]. The fluctuation-corrected universal power laws governing the vicinity of the phase transition can be extracted by renormalization group methods (reviewed for directed percolation in Ref. [39]). Table 1 compares the analytic results obtained in an  $\epsilon$  expansion about the critical dimension ( $\epsilon = 4 - d$ ) with the critical exponent values measured in Monte Carlo computer simulations [33, 34].

According to a conjecture originally formulated by Janssen and Grassberger, any continuous nonequilibrium phase transition from an active to an absorbing state in a system governed by Markovian stochastic dynamics that is decoupled from any other slow variable, and in the absence of special additional symmetries or quenched randomness, should in fact fall in the directed percolation universality class (Janssen 1981 [38], Grassberger 1982 [40]). This statement has indeed been confirmed in a large variety of model systems (many

**Table 1. Field-theoretic Methods.** Comparison of the values for the critical exponents of the directed percolation universality class measured in Monte Carlo simulations with the analytic renormalization group results within the  $\epsilon = 4 - d$  expansion:  $\xi$  denotes the correlation length,  $t_c$  the characteristic relaxation time,  $a_s$  the saturation density in the active state, and  $a_c(t)$  the critical density decay law.

Scaling exponent	$d = 1$	$d = 2$	$d = 4 - \epsilon$
$\xi \sim  \tau ^{-\nu}$	$\nu \approx 1.100$	$\nu \approx 0.735$	$\nu = 1/2 + \epsilon/16 + O(\epsilon^2)$
$t_c \sim \xi^z \sim  \tau ^{-z\nu}$	$z \approx 1.576$	$z \approx 1.73$	$z = 2 - \epsilon/12 + O(\epsilon^2)$
$a_s \sim  \tau ^\beta$	$\beta \approx 0.2765$	$\beta \approx 0.584$	$\beta = 1 - \epsilon/6 + O(\epsilon^2)$
$a_c(t) \sim t^{-\alpha}$	$\alpha \approx 0.160$	$\alpha \approx 0.46$	$\alpha = 1 - \epsilon/4 + O(\epsilon^2)$

examples are listed in Refs. [33, 34]). It even pertains to multi-species generalizations (Janssen 2001 [41]), and applies for instance to the predator extinction threshold in the stochastic Lotka–Volterra model with restricted site occupation numbers mentioned in section 2.2 [4].

## 5 Stochastic differential equations

This section explains how dynamics governed by *Langevin-type stochastic differential equations* can be represented through a field-theoretic formalism [14]–[16]. Such a description is especially useful to capture the effects of external noise on the temporal evolution of the relevant quantities under consideration, which encompasses the case of thermal noise induced by the coupling to a heat bath in thermal equilibrium at temperature  $T$ . The underlying assumption in this approach is that there exists a natural *separation of time scales* between the slow variables  $S_i$ , and all other degrees of freedom  $\zeta_i$  which in comparison fluctuate rapidly, and are therefore summarily gathered in zero-mean noise terms, assumed to be uncorrelated in space and time,

$$\langle \zeta_i(x, t) \rangle = 0, \quad \langle \zeta_i(x, t) \zeta_j(x', t') \rangle = 2L_{ij}[S_i] \delta(x - x') \delta(t - t'). \quad (30)$$

Here, the noise correlator  $2L_{ij}[S_i]$  may be a function of the slow system variables  $S_i$ , and also contain operators such as spatial derivatives. A general set of coupled Langevin-type stochastic differential equations then takes the form

$$\frac{\partial S_i(t)}{\partial t} = F_i[S_i] + \zeta_i, \quad (31)$$

where we may decompose the ‘systematic forces’ into reversible terms of microscopic origin and relaxational contributions that are induced by the noise and drive the system towards its stationary state (see below), i.e.:  $F_i[S_i] = F_i^{\text{rev}}[S_i] + F_i^{\text{rel}}[S_i]$ . Both ingredients may contain nonlinear terms as well as mode couplings between different variables. Again, we first introduce the abstract formalism, and then proceed to discuss relaxation to thermal equilibrium as well as some examples for nonequilibrium Langevin dynamics.

### 5.1 Field theory representation of Langevin equations

The shortest and most general route towards a field theory representation of the Langevin dynamics (31) with noise correlations (30) starts with one of the most elaborate ways to expand unity, namely through a product of functional delta functions (for the sake of compact notations, we immediately employ a functional integration language, but in the end all the path integrals are defined through appropriate discretizations in space and time):

$$\begin{aligned} 1 &= \int \prod_i \mathcal{D}[S_i] \prod_{(x,t)} \delta \left( \frac{\partial S_i(x,t)}{\partial t} - F_i[S_i](x,t) - \zeta_i(x,t) \right) \\ &= \int \prod_i \mathcal{D}[i\tilde{S}_i] \mathcal{D}[S_i] \exp \left[ - \int d^d x \int dt \sum_i \tilde{S}_i \left( \frac{\partial S_i}{\partial t} - F_i[S_i] - \zeta_i \right) \right]. \end{aligned} \quad (32)$$

In the second line we have used the Fourier representation of the (functional) delta distribution by means of the purely imaginary auxiliary variables  $\tilde{S}_i$  (also called Martin–Siggia–Rose response fields [42]). Next we require the explicit form of the noise probability distribution that generates the correlations (30); for simplicity, we may employ the Gaussian

$$\mathcal{W}[\zeta_i] \propto \exp \left[ - \frac{1}{4} \int d^d x \int_0^{t_f} dt \sum_{ij} \zeta_i(x,t) [L_{ij}^{-1} \zeta_j(x,t)] \right]. \quad (33)$$

Inserting the identity (32) and the probability distribution (33) into the desired stochastic noise average of any observable  $\mathcal{O}[S_i]$ , we arrive at

$$\begin{aligned} \langle \mathcal{O}[S_i] \rangle_\zeta &\propto \int \prod_i \mathcal{D}[i\tilde{S}_i] \mathcal{D}[S_i] \exp \left[ - \int d^d x \int dt \sum_i \tilde{S}_i \left( \frac{\partial S_i}{\partial t} - F_i[S_i] \right) \right] \mathcal{O}[S_i] \\ &\times \int \prod_i \mathcal{D}[\zeta_i] \exp \left( - \int d^d x \int dt \sum_i \left[ \frac{1}{4} \zeta_i \sum_j L_{ij}^{-1} \zeta_j - \tilde{S}_i \zeta_i \right] \right). \end{aligned} \quad (34)$$

Subsequently evaluating the Gaussian integrals over the noise  $\zeta_i$  yields at last

$$\langle \mathcal{O}[S_i] \rangle_\zeta = \int \prod_i \mathcal{D}[S_i] \mathcal{O}[S_i] \mathcal{P}[S_i], \quad \mathcal{P}[S_i] \propto \int \prod_i \mathcal{D}[i\tilde{S}_i] e^{-\mathcal{A}[\tilde{S}_i, S_i]}, \quad (35)$$

with the statistical weight governed by the Janssen–De Dominicis ‘response’ functional [14, 15]

$$\mathcal{A}[\tilde{S}_i, S_i] = \int d^d x \int_0^{t_f} dt \sum_i \left[ \tilde{S}_i \left( \frac{\partial S_i}{\partial t} - F_i[S] \right) - \tilde{S}_i \sum_j L_{ij} \tilde{S}_j \right]. \quad (36)$$

It should be noted that in the above manipulations, we have omitted the functional determinant from the variable change  $\{\zeta_i\} \rightarrow \{S_i\}$ . This step can be

justified through applying a forward (Itô) discretization (for technical details, see Refs. [43, 16, 27]). Normalization implies  $\int \prod_i \mathcal{D}[i\tilde{S}_i] \mathcal{D}[S_i] e^{-\mathcal{A}[\tilde{S}_i, S_i]} = 1$ . The first term in the action (36) encodes the temporal evolution according to the systematic terms in the Langevin equations (31), whereas the second term specifies the noise correlations (30). Since the auxiliary fields appear only quadratically, they could be eliminated via completing the squares and Gaussian integrations. This results in the equivalent Onsager–Machlup functional which however contains squares of the nonlinear terms and the inverse of the noise correlator operators; the form (36) is therefore usually more convenient for practical purposes. The Janssen–De Dominicis functional (36) takes the form of a  $(d+1)$ -dimensional statistical field theory with again *two* independent sets of fields  $S_i$  and  $\tilde{S}_i$ . It may serve as a starting point for systematic approximation schemes including perturbative expansions, and subsequent renormalization group treatments. Causality is properly incorporated in this formalism which has important technical implications [43, 16, 27].

## 5.2 Thermal equilibrium and relaxational critical dynamics

Consider the dynamics of a system that following some external perturbation relaxes towards thermal equilibrium governed by the canonical Boltzmann distribution at fixed temperature  $T$ ,

$$\mathcal{P}_{\text{eq}}[S_i] = \frac{1}{\mathcal{Z}(T)} \exp(-\mathcal{H}[S_i]/k_{\text{B}}T) . \quad (37)$$

The relaxational term in the Langevin equation (31) can then be specified as

$$F_i^{\text{rel}}[S_i] = -\lambda_i \frac{\delta \mathcal{H}[S_i]}{\delta S_i} , \quad (38)$$

with Onsager coefficients  $\lambda_i$ ; for nonconserved fields,  $\lambda_i$  is a positive relaxation rate. On the other hand, if the variable  $S_i$  is a conserved quantity (such as the energy density), there is an associated continuity equation  $\partial S_i / \partial t + \nabla \cdot J_i = 0$ , with a conserved current that is typically given by a gradient of the field  $S_i$ :  $J_i = -D_i \nabla S_i + \dots$ ; as a consequence, the fluctuations of the fields  $S_i$  will relax diffusively with diffusivity  $D_i$ , and  $\lambda_i = -D_i \nabla^2$  becomes a spatial Laplacian.

In order for  $\mathcal{P}(t) \rightarrow \mathcal{P}_{\text{eq}}$  as  $t \rightarrow \infty$ , the stochastic Langevin dynamics needs to satisfy *two* conditions, which can be inferred from the associated Fokker–Planck equation [44, 27]. First, the reversible probability current is required to be divergence-free in the space spanned by the fields  $S_i$ :

$$\int d^d x \sum_i \frac{\delta}{\delta S_i(x)} \left( F_i^{\text{rev}}[S_i] e^{-\mathcal{H}[S_i]/k_{\text{B}}T} \right) = 0 . \quad (39)$$

This condition severely constrains the reversible force terms. For example, for a system whose microscopic time evolution is determined through the

Poisson brackets  $Q_{ij}(x, x') = \{S_i(x), S_j(x')\} = -Q_{ji}(x', x)$  (to be replaced by commutators in quantum mechanics), one finds for the reversible mode-coupling terms [44]

$$F_i^{\text{rev}}[S_i](x) = - \int d^d x' \sum_j \left[ Q_{ij}(x, x') \frac{\delta \mathcal{H}[S_i]}{\delta S_j(x')} - k_B T \frac{\delta Q_{ij}(x, x')}{\delta S_j(x')} \right]. \quad (40)$$

Second, the noise correlator in Eq. (30) must be related to the Onsager relaxation coefficients through the Einstein relation

$$L_{ij} = k_B T \lambda_i \delta_{ij}. \quad (41)$$

To provide a specific example, we focus on the case of purely relaxational dynamics (i.e., reversible force terms are absent entirely), with the (mesoscopic) Hamiltonian given by the Ginzburg–Landau–Wilson free energy that describes second-order phase transitions in thermal equilibrium for an  $n$ -component order parameter  $S_i$ ,  $i = 1, \dots, N$  [6]–[13]:

$$\mathcal{H}[S_i] = \int d^d x \sum_{i=1}^N \left[ \frac{r}{2} [S_i(x)]^2 + \frac{1}{2} [\nabla S_i(x)]^2 + \frac{u}{4!} [S_i(x)]^2 \sum_{j=1}^N [S_j(x)]^2 \right], \quad (42)$$

where the control parameter  $r \propto T - T_c$  changes sign at the critical temperature  $T_c$ , and the positive constant  $u$  governs the strength of the nonlinearity. If we assume that the order parameter itself is not conserved under the dynamics, the associated response functional reads

$$\mathcal{A}[\tilde{S}_i, S_i] = \int d^d x \int dt \sum_i \tilde{S}_i \left( \frac{\partial}{\partial t} + \lambda_i \frac{\delta \mathcal{H}[S_i]}{\delta S_i} - k_B T \lambda_i \tilde{S}_i \right). \quad (43)$$

This case is frequently referred to as model A critical dynamics [45]. For a diffusively relaxing conserved field, termed model B in the classification of Ref. [45], one has instead

$$\mathcal{A}[\tilde{S}_i, S_i] = \int d^d x \int dt \sum_i \tilde{S}_i \left( \frac{\partial}{\partial t} - D_i \nabla^2 \frac{\delta \mathcal{H}[S_i]}{\delta S_i} + k_B T D_i \nabla^2 \tilde{S}_i \right). \quad (44)$$

Consider now the external fields  $h_i$  that are thermodynamically conjugate to the mesoscopic variables  $S_i$ , i.e.,  $\mathcal{H}(h_i) = \mathcal{H}(h_i = 0) - \int d^d x \sum_i h_i(x) S_i(x)$ . For the simple relaxational models (43) and (44), we may thus immediately relate the dynamic susceptibility to two-point correlation functions that involve the auxiliary fields  $\tilde{S}_i$  [43], namely

$$\chi_{ij}(x - x', t - t') = \left. \frac{\delta \langle S_i(x, t) \rangle}{\delta h_j(x', t')} \right|_{h_i=0} = k_B T \lambda_i \langle S_i(x, t) \tilde{S}_j(x', t') \rangle \quad (45)$$

for nonconserved fields, while for model B dynamics

$$\chi_{ij}(x - x', t - t') = -k_B T D_i \left\langle S_i(x, t) \nabla^2 \tilde{S}_j(x', t') \right\rangle . \quad (46)$$

Finally, in thermal equilibrium the dynamic response and correlation functions are related through the fluctuation–dissipation theorem [43]

$$\chi_{ij}(x - x', t - t') = \Theta(t - t') \frac{\partial}{\partial t'} \langle S_i(x, t) S_j(x', t') \rangle . \quad (47)$$

### 5.3 Driven diffusive systems and interface growth

We close this section by listing a few intriguing examples for Langevin systems that describe genuine out-of-equilibrium dynamics. First, consider a driven diffusive lattice gas (an overview is provided in Ref. [46]), namely a particle system with conserved total density with biased diffusion in a specified (‘||’) direction. The coarse-grained Langevin equation for the scalar density fluctuations thus becomes spatially anisotropic [47, 48],

$$\frac{\partial S(x, t)}{\partial t} = D \left( \nabla_{\perp}^2 + c \nabla_{\parallel}^2 \right) S(x, t) + \frac{Dg}{2} \nabla_{\parallel} S(x, t)^2 + \zeta(x, t) , \quad (48)$$

and similarly for the conserved noise with  $\langle \zeta \rangle = 0$ ,

$$\langle \zeta(x, t) \zeta(x', t') \rangle = -2D \left( \nabla_{\perp}^2 + \tilde{c} \nabla_{\parallel}^2 \right) \delta(x - x') \delta(t - t') . \quad (49)$$

Notice that the drive term  $\propto g$  breaks both the system’s spatial reflection symmetry as well as the Ising symmetry  $S \rightarrow -S$ . In one dimension, Eq. (48) coincides with the noisy Burgers equation [49], and since in this case (only) the condition (39) is satisfied, effectively represents a system with equilibrium dynamics. The corresponding Janssen–De Dominicis response functional reads

$$\mathcal{A}[\tilde{S}, S] = \int d^d x \int dt \tilde{S} \left[ \frac{\partial S}{\partial t} - D \left( \nabla_{\perp}^2 + c \nabla_{\parallel}^2 \right) S + D \left( \nabla_{\perp}^2 + \tilde{c} \nabla_{\parallel}^2 \right) \tilde{S} - \frac{Dg}{2} \nabla_{\parallel} S^2 \right] . \quad (50)$$

It describes a ‘massless’ theory, hence we expect the system to generically display scale-invariant features, without the need to tune to a special point in parameter space. The large-scale scaling properties can be analyzed by means of the dynamic renormalization group [47, 48].

Another famous example for generic scale invariance emerging in a nonequilibrium system is curvature-driven interface growth, as captured by the Kardar–Parisi–Zhang equation [50]

$$\frac{\partial S(x, t)}{\partial t} = D \nabla^2 S(x, t) + \frac{Dg}{2} [\nabla S(x, t)]^2 + \zeta(x, t) , \quad (51)$$

with again  $\langle \zeta \rangle = 0$  and the noise correlations

$$\langle \zeta(x, t) \zeta(x', t') \rangle = 2D \delta(x - x') \delta(t - t') . \quad (52)$$

(For more details and intriguing variants, see e.g. Refs. [51]-[53].) The associated field theory action

$$\mathcal{A}[\tilde{S}, S] = \int d^d x \int dt \left[ \tilde{S} \left( \frac{\partial S}{\partial t} - D \nabla^2 S - \frac{Dg}{2} [\nabla S]^2 \right) - D \tilde{S}^2 \right] \quad (53)$$

encodes surprisingly rich behavior including a kinetic roughening transition separating two distinct scaling regimes in dimensions  $d > 2$  [51]-[53].

## 6 Future directions

The rich phenomenology in many complex systems is only inadequately captured within widely used mean-field approximations, wherein both statistical fluctuations and correlations induced by the subunits' interactions or the system's kinetics are neglected. Modern computational techniques, empowered by recent vast improvements in data storage and tact frequencies, as well as the development of clever algorithms, are clearly invaluable in the theoretical study of model systems displaying the hallmark features of complexity. Yet in order to gain a deeper understanding and to maintain control over the typically rather large parameter space, numerical investigations need to be supplemented by analytical approaches. The field-theoretic methods described in this article represent a powerful set of tools to systematically include fluctuations and correlations in the mathematical description of complex stochastic dynamical systems composed of many interacting degrees of freedom. They have already been very fruitful in studying the intriguing physics of highly correlated and strongly fluctuating many-particle systems. Aside from many important quantitative results, they have provided the basis for our fundamental understanding of the emergence of universal macroscopic features.

At the time of writing, the transfer of field-theoretic methods to problems in chemistry, biology, and other fields such as sociology has certainly been initiated, but is still limited to rather few and isolated case studies. This is understandable, since becoming acquainted with the intricate technicalities of the field theory formalism requires considerable effort. Also, whereas it is straightforward to write down the actions corresponding the stochastic processes defined via microscopic classical discrete master or mesoscopic Langevin equations, it is usually not that easy to properly extract the desired information about large-scale structures and long-time asymptotics. Yet if successful, one tends to gain insights that are not accessible by any other means. I therefore anticipate that the now well-developed methods of quantum and statistical field theory, with their extensions to stochastic dynamics, will find ample successful applications in many different areas of complexity science. Naturally, further approximation schemes and other methods tailored to the questions at hand will have to be developed, and novel concepts be devised. I look forward to learning about and hopefully also participating in these exciting future developments.

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