Field theory for reaction-diffusion processes with hard-core particles

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(Received 28 September 2000; published 25 January 2001)

We show how to build up a systematic bosonic field theory for a general reaction-diffusion process involving *hard-core* particles in arbitrary dimension. We discuss a recent approach proposed by Park, Kim, and Park [Phys. Rev. E **62**, 7642 (2000)]. As a test bench for our method, we show how to recover the equivalence between asymmetric diffusion of excluding particles and the noisy Burgers equation.

DOI: 10.1103/PhysRevE.63.022101 PACS number(s): 05.40.−a

I. INTRODUCTION

A general formalism to describe nonequilibrium statistical physics is still lacking, but recent progress has been achieved on the important issue of the description of collective phenomena in such systems (phase transitions in nonequilibrium steady-states [1], the emergence of long-range correlations in driven systems [2], cellular automata [3], and self-organized criticality [4]). Indeed, steps forward have been made in the last two decades in that direction by exploiting the formal analogy of their field-theoretic formulation with static critical phenomena. Of course, numerical approaches and exact solutions have played an equally important role, but this paper will deliberately ignore those aspects. The beauty of the field-theoretic formulation—when available—is that, combined with a renormalization-group analysis, it provides the theorist with a systematic analytic tool for the calculation of physical observables in the scaling regimes of interest. However, a vast category of reaction-diffusion processes, cellular automata, driven lattice gases, and other related stochastic models fail to be exactly mapped onto continuous field theories [5]. This difficulty is due to the fact that the integer degrees of freedom (often particle numbers) usually have an integer upper limit that prevents one from exploiting the familiar mapping first introduced by Doi [6] and recently revived by Cardy [7]. For instance, in a reaction-diffusion process with mutually excluding particles, local particle numbers are 0 or 1, but one might imagine other processes with other similar constraints (e.g., the contact threshold transfer process defined by Rossi *et al.* [8] in which a given site is occupied by no more than two particles). In some instances, the exclusion constraint can be phenomenologically accounted for, as done, e.g., by Zia and Schmittmann [2] when they build up the effective Langevin equations to describe the dynamics of driven-diffusive systems. Very often the evolution operator can be exactly mapped on a quantum spin chain. But it is only in one space dimension that (in favorable cases) one can exploit the toolbox of integrable systems [9] [local particle numbers usually restricted to 0 and 1, little being known [10] on spin-1 (and higher) chains for stochastic problems]. A coveted goal is therefore to be able to build up a systematic and exact field-theoretic path-integral formulation that can, at least formally, account for limitations in local particle numbers.

Several attempts have been made to incorporate the exclusion constraint into a field theory of a standard type. As already mentioned, one may achieve this goal by phenomenologically exploiting the physical knowledge of the system (Zia and Schmittmann [2] or Cardy [11]), but this is by no means exact, and can in general only be implemented safely in high space dimension. Directly in dimension 1, other approaches exist, such as that proposed by Cardy [12] and Brunel *et al.* [13], or by Mobilia and Bares [14]. In the former the authors succeeded in constructing a field theory in a systematic way, but of fermionic type, which unfortunately proved, from a technical view, rather difficult to analyze, while the latter, though efficient in the pair annihilation reaction, seems difficult to extend to other processes.

In what follows we shall present the derivation of the path-integral formulation for systems of mutually excluding particles of a single species. Where appropriate we will also indicate how to extend the theory to cope with several species or other constraints on local particle numbers. We shall illustrate how the mapping works on the case of asymmetric diffusion, and how one can recover the equivalence with the noisy Burgers equation.

II. HARD-CORE PARTICLES USING A BOSONIC FORMULATION

A. Master equation and bosonic formalism

The evolution of a configuration $n\equiv\{n_i\}$ of local particle numbers is encoded in a master equation for the probability $P(n,t)$ to observe configuration n at time t. The master equation for $P(n,t)$ is equivalent to an evolution equation for the state vector $|\Psi(t)\rangle=\Sigma_n P(n,t)|n\rangle$, which we write in the form

$$\partial_t|\Psi\rangle=-\hat{H}|\Psi\rangle. \tag{1}$$

The operator $\hat{H}$, which acts on the space spanned by the configuration vectors $|n\rangle$, is usually easily expressed in terms of bosonic creation and annihilation operators $a_i^\dagger, a_i$ ($[a_i,a_j^\dagger]=\delta_{ij},[a_i,a_j]=0$). This is true for reaction-diffusion processes involving *bosonic particles*; that is, without exclusion, for which bosonic operators are particularly well-suited, but this is also true when particles exclude each other. Nevertheless in the latter situation one should not expect that $\hat{H}$ will be a polynomial in terms of the $a_i, a_j^\dagger$, while it indeed is in the former. We confine the subsequent analysis to the dynamics of hard-core (i.e., mutually excluding particles) undergoing diffusion and reaction processes.

B. Evolution operators for some elementary processes

In order to deal with the exclusion constraint we introduce the operator $\delta_{\hat{n},m}$ defined by

$$\delta_{\hat{n},m}|m'\rangle = \delta_{m',m}|m'\rangle, \tag{2}$$

where $|m\rangle$ denotes a single site state. We now give two examples. The evolution operator for one-dimensional asymmetric diffusion in the presence of hard-core interactions reads

$$\hat{H}_{\rm diff} = \sum_i \left[\left(D+\frac{v}{2}\right)(1-a_i a_{i+1}^\dagger)\,\delta_{\hat{n}_i,1}\delta_{\hat{n}_{i+1},0} + \left(D-\frac{v}{2}\right)(1-a_i^\dagger a_{i+1})\,\delta_{\hat{n}_i,0}\delta_{\hat{n}_{i+1},1}\right], \tag{3}$$

where $D+v/2$ (respectively, $D-v/2$) is the hopping rate to the right (respectively, to the left).

For the simple $A+A\xrightarrow{k}\varnothing$ annihilation reaction of nearest-neighbor particles, one finds

$$\hat{H}_k = k\sum_i \left[(1-a_i^\dagger a_{i+1}^\dagger)\,\delta_{\hat{n}_i,1}\delta_{\hat{n}_{i+1},1}\right]. \tag{4}$$

Extension to two-species annihilation is straighforward since bosonic operators pertaining to distinct species commute.

C. Passing to a coherent-state representation

In order to pass to a path-integral formulation, it is sufficient to follow the steps described in [15] (for a thorough and pedagogical introduction we refer the reader to the review by Mattis and Glasser [16]). The result of those steps can be summarized as follows. There exists an action $S[\hat{\phi},\phi]$ such that physical observables can be expressed as path integrals over the complex fields $\hat{\phi}_i(t),\phi_i(t)$ of functions of those fields, weighted by $\exp(-S)$. We denote by $[0,t_f]$ the time interval over which the process is studied. The action S has the form

$$S = -\sum_i \phi_i(t_f) + \int_0^{t_f} dt\left(\sum_i \hat{\phi}_i(t)\partial_t\phi_i + H[\hat{\phi},\phi]\right), \tag{5}$$

where

$$H[\hat{\phi},\phi] = \frac{\langle\phi|\hat{H}|\phi\rangle}{\langle\phi|\phi\rangle}, \tag{6}$$

in which the notation $|\phi\rangle = \otimes_i|\phi_i(t)\rangle$ denotes the tensor product of the coherent states associated with each creator and annihilator $a_i^\dagger, a_i$ with eigenvalue $\phi_i(t)$ [and $\hat{\phi}_i(t)$ denotes the complex conjugate of $\phi_i(t)$]. In order to evaluate the quantity $\langle\phi|\hat{H}|\phi\rangle/\langle\phi|\phi\rangle$, one normal orders $\hat{H}$ and then simply replaces the a_i's by $\phi_i(t)$ and the $a_i^\dagger$'s by $\hat{\phi}_i(t)$. Hence the only difficulty is to be able to normal order such an operator as $\delta_{\hat{n},m}$ (possibly multiplied by a's or $a^\dagger$'s). This can be done rather easily in several ways. One of them is simply to normal order $\mathrm{e}^{iu\hat{n}}$ then make use of the integral representation

$$\delta_{\hat{n},m} = \int_{-\pi}^{\pi}\frac{du}{2\pi}e^{iu(\hat{n}-m)}.$$

Normal ordering $\mathrm{e}^{iu\hat{n}}$ is done by expanding the exponential and looking at each term in the series. It is amusing to note that

$$:e^{iu\hat{n}}: = \sum_{\ell=0}^{\infty}\frac{(iu)^\ell}{\ell!}\sum_{j=1}^{\ell} s_{j,\ell}\,a^{\dagger j}a^j, \tag{7}$$

where the coefficients $s_{j,\ell}$ are the Stirling numbers of the second kind $[s_{j,\ell}=(1/n!)(\mathrm{d}^n/\mathrm{d}x^n)(\mathrm{e}^x-1)^j|_{x=0}$ is the number of ways a set with ℓ elements can be partitioned into j disjoint, nonempty subsets]. Similarly, one finds that

$$:\mathrm{e}^{iua^\dagger a}a^\dagger: = a^\dagger:\mathrm{e}^{iua^\dagger a}: + \sum_n \frac{(iu)^n}{n!}\sum_j j s_{j,n}a^{\dagger j}a^{j-1}. \tag{8}$$

Once in their normal-ordered form, the operators a and $a^\dagger$ in Eqs. (7) and (8) can be replaced by their coherent-state eigenvalues. For instance,

$$\langle\phi|e^{iu\hat{n}}|\phi\rangle = \sum_{\ell=0}^{+\infty}\frac{(iu)^\ell}{\ell!}\sum_{j=1}^{\ell}s_{j,\ell}\hat{\phi}^j\phi^j = e^{\hat{\phi}\phi(\mathrm{e}^{iu}-1)}, \tag{9}$$

so that

$$\langle\phi|\,\delta_{\hat{n},0}|\phi\rangle = \int_{-\pi}^{\pi}\frac{\mathrm{d}u}{2\pi}e^{\hat{\phi}\phi(\mathrm{e}^{iu}-1)} = e^{-\hat{\phi}\phi}. \tag{10}$$

Similar manipulations lead to the dictionary

$$\begin{aligned}\langle\phi|a^\dagger\delta_{\hat{n},m}|\phi\rangle &= \frac{1}{m!}\hat{\phi}(\hat{\phi}\phi)^m e^{-\hat{\phi}\phi},\\ \langle\phi|\,\delta_{\hat{n},m}|\phi\rangle &= \frac{1}{m!}(\hat{\phi}\phi)^m e^{-\hat{\phi}\phi},\\ \langle\phi|a\,\delta_{\hat{n},m}|\phi\rangle &= \phi\frac{1}{(m-1)!}(\hat{\phi}\phi)^{m-1}e^{-\hat{\phi}\phi}\\ &(=0 \ \text{ if } \ m=0).\end{aligned} \tag{11}$$

In a reaction-diffusion process with hard-core particles, only the formulas for $m=0$ or 1 will be needed. Formulas with higher powers of the a's or $a^\dagger$'s are derived in a similar way.

For example, the action for the annihilation process described by the evolution operator of Eq. (4) reads

$$S = k\int dt\sum_i \left[(\hat{\phi}_i\hat{\phi}_{i+1}-1)\phi_i\phi_{i+1}e^{-\hat{\phi}_i\phi_i-\hat{\phi}_{i+1}\phi_{i+1}}\right]. \tag{12}$$

Extensions to several species pose no new problem. A final remark: when studying a process that conserves the parity of the instantaneous total number of particles $N(t)$ in the system, the following quantity is conserved:

$$\langle(-1)^{N(t)}\rangle=\langle e^{i\pi N(t)}\rangle=\langle \mathbf{p}|e^{i\pi\sum_i \hat{n}_i}|\Psi\rangle, \qquad (13)$$

where $\langle \mathbf{p}|\equiv\langle 0|e^{\Sigma_i a_i}$ denotes the projection state [15], which is also a coherent state with eigenvalue 1, so that, using that $\langle 1|e^{i\pi\hat{n}_i}|\phi_i\rangle=e^{\phi_i(e^{i\pi}-1)}$, we find

$$\langle(-1)^{N(t)}\rangle=\left\langle e^{-2\sum_i \phi_i(t)}\right\rangle=\text{const.} \qquad (14)$$

This is a way of characterizing parity by means of a well-defined observable. We refer the reader to Deloubrière and Hilhorst [17] for further comments in the context of the pair annihilation reaction.

D. The Park, Kim, and Park approach

It is well-known [18] that for reaction-diffusion processes involving bosonic particles (which is not the case in [19]) it is possible to write a partial-differential equation for some continuous random variable ρ_i (the mapping fails for hard-core particles). The first moment of ρ_i equals the average local particle number $\langle n_i\rangle$ (which makes it tempting to identify ρ_i with a fluctuating density). However, higher moments of ρ_i do not coincide with those of n_i (though they can be related). This partial-differential equation takes a Fokker-Planck form (i.e., is of order 2) only when the microscopic reactions involve at most two particles.

We now refer to the article [19] in which the authors have presented an alternative route to derive a path-integral formulation for the dynamics of hard-core particle systems. Particle numbers are discrete variables, so that there is no Fokker-Planck equation for them. In their Eq. (7) they write a Fokker-Planck equation for some continuous random variable ρ_i, which, as we have said, is not correct without further approximation. This error is not related to the necessity of implementing the hard-core constraint or not. Such a Fokker-Planck equation simply does not exist. References and further comments can be found in the book by Gardiner [18] or in Deloubrière and Hilhorst [17].

III. AN EXAMPLE: ASYMMETRIC DIFFUSION OF HARD-CORE PARTICLES AND THE NOISY BURGERS EQUATION

As an example we recover the noisy Burgers equation by going to the continuous limit in the asymmetric diffusion of a system of hard-core particles. While this equivalence is certainly not new [20–22], we use it as a test bench for the method. It should be mentioned that this derivation of the noisy Burgers equation is the first one that starts from an exact mapping.

A. Action

Again, for notational simplicity, we restrict the analysis to one space dimension. We consider diffusion with a hopping rate to the right $D+v/2$ and a hopping rate to the left $D-v/2$. The evolution operator for such asymmetric diffusion in the presence of hard-core interactions is that of Eq. (3). Using the dictionary equation (11) we find that the corresponding action reads

$$\begin{aligned}S[\hat{\phi},\phi]=\int dt\sum_i\bigg[&\hat{\phi}_i\partial_t\phi_i\\&+\left(D+\frac{v}{2}\right)(\hat{\phi}_i-\hat{\phi}_{i+1})\phi_i e^{-\hat{\phi}_i\phi_i-\hat{\phi}_{i+1}\phi_{i+1}}\\&+\left(D-\frac{v}{2}\right)(\hat{\phi}_i-\hat{\phi}_{i-1})\phi_i e^{-\hat{\phi}_i\phi_i-\hat{\phi}_{i-1}\phi_{i-1}}\bigg].\end{aligned} \qquad (15)$$

No approximation was made and the action equation (15) is fully exact. Without the exponential factors Eq. (15) would yield the usual action of asymmetric diffusion for bosonic particles. Here, owing to the presence of the nonlinear interaction terms (the exponentials), there is no Galilean transformation that eliminates the drift-dependent terms.

B. Recovering the noisy Burgers equation in the continuous limit

In this paragraph, we shall show that expanding naively the action equation (15) leads to the noisy Burgers equation for the density fluctuations, as it should. We perform the change of fields [23] $\phi_i=(\rho+\psi_i)e^{-\overline{\psi}_i}$, $\hat{\phi}_i=e^{\overline{\psi}_i}$. Now we expand the action in powers of the new fields $\overline{\psi}_i$ and ψ_i (the latter represents a fluctuation of the density with respect to its average value ρ). We also assume that the fields have slow space variations, and take the limit of a continuous space. The resulting action reads

$$\begin{aligned}S=\int dtdx[&\overline{\psi}(\partial_t+v\partial_x-D\partial_x^2)\psi-g_1(\partial_x\overline{\psi})^2\\&-g_2\overline{\psi}\psi\partial_x\psi+\cdots],\end{aligned} \qquad (16)$$

where the constants g_1,g_2 are positive functions of the microscopic details of the model (diffusion constant, drift velocity, lattice spacing, average density). The dots stand for higher polynomial or higher derivative terms. The action equation (16) for the fields $\overline{\psi},\psi$ is equivalent to $\psi(x,t)$ satisfying the noisy Burgers equation [22]. Hence, up to terms that are irrelevant in the scaling limit [see Janssen and Schmittmann [22] for a renormalization-group analysis of the action equation (16)], we have recovered the equivalence between asymmetric diffusion of hard-core particles and the noisy Burgers equation. As a final remark, we would like to emphasize that we have not resorted to any phenomenological arguments, and that our derivation is completely systematic—the first one of this sort. This feature is particularly encouraging since we have in mind the application of the formalism to other less studied processes.

IV. CONCLUSIONS

We have shown how to build up a field-theoretic formalism that takes into account in a systematic fashion the effect of exclusion in *d*-dimensional reaction-diffusion processes. We have exemplified the formalism on the case of asymmetric diffusion, thus recovering the noisy Burgers equation. We now have a tool to take up any reaction-diffusion process in which one, or all species, diffuse with a drift, such as the $A+B\rightarrow\emptyset$ reaction, for which it is conjectured that exclusion changes the universality class of the scaling behavior. The $A+B\rightarrow\emptyset$ reaction-diffusion process with drift is certainly the first system that should be looked at using the present approach. However, great care must be paid to naive expansions of exponential interaction terms, and the feasibility of such a procedure must be investigated in each particular case. The method presented here opens the door to the study of reaction-diffusion processes in which exclusion is conjectured to play a crucial role, such as in the N species branching annihilating random walks recently described by Kwon *et al.* [24].

ACKNOWLEDGMENTS

The author would like to thank Henk Hilhorst, Uwe Täuber, and Martin Howard without whom this approach would not have been elaborated, and would like to thank Gunter Schütz for communicating Ref. [9] prior to publication.

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