

Exact density profile of a stochastic reaction-diffusion process

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We calculate exactly the time dependent density profile of a one-dimensional stochastic reaction-diffusion process of hard-core particles subjected to the reactions $AA \rightleftharpoons OO$ and $AO \rightleftharpoons OA$. The solution is based on the fundamental property that the evolution operator, defined over an appropriate vector space, transforms vectors with n kinks into vectors with n or $n+2$ kinks, only. In this space, a basis vector is represented by a string of plus and minus signs and a kink is defined as a pair of opposite signs. The exact time dependent profiles are calculated for the cases of uncorrelated initial states that are translational invariant as well as initial states that are inhomogeneous in space. [S1063-651X(99)01409-9]

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I. INTRODUCTION

The connection between stochastic reaction-diffusion systems defined on a lattice and quantum spin models [1–18] has been found to be fruitful for both areas of research. The techniques developed for the investigation of quantum spin models can be used in the study of reaction-diffusion systems and, conversely, some results known for the latter might provide information for quantum spin models. The best known example of such a connection is related to the symmetric diffusion of classical hard-core particles on a lattice, or symmetric exclusion process, whose evolution operator can be mapped into the quantum spin-1/2 ferromagnetic Heisenberg Hamiltonian. For a review on the uses of quantum theory in diffusion-limited reactions see the recent work by Mattis and Glasser [19].

In general for a stochastic system of hard-core particles, in which no more than one particle can be present on a site, described by a master equation, it is possible to map the corresponding evolution operator into a generalized spin-1/2 Heisenberg operator that need not be Hermitian. In fact, only when the stochastic process, in the stationary state, has detailed balance (or equivalently microscopic reversibility) can it be brought into a Hermitian form. Usually, the quantum Heisenberg operator is written in a representation in which an occupied site is associated to a spinor $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and an empty site by a spinor $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$. In one dimension it is possible to obtain, in certain cases, an exact solution by means of techniques such as the use of the Bethe ansatz and the mapping into a free fermion model by a Jordan-Wigner transformation.

In this paper we consider a reaction-diffusion stochastic process occurring on a one-dimensional lattice in which each site may be occupied by at most one particle (A) or may be empty (O). The process is composed of the following four reactions: (a) $OO \rightarrow AA$, creation of two particles with rate Γ_0 , (b) $OA \rightarrow AO$, diffusion to the left with rate Γ_1 , (c) $AO \rightarrow OA$, diffusion to the right with rate Γ_2 , and (d) $AA \rightarrow OO$, annihilation of two particles with rate Γ_3 . Such a reaction-diffusion process and particular cases of it have been treated by the use of a quantum formalism [1–10] and also by other approaches [20–26]. When the transition rates obey the *free fermion* condition [5,6], $\Gamma_0 + \Gamma_3 = \Gamma_1 + \Gamma_2$, the

evolution operator can be mapped into a Heisenberg operator which turns out to be integrable by a Jordan-Wigner transformation [5,6]. From the solution it is possible to derive correlation functions and the density profile as functions of time. When $\Gamma_0 = 0$ and $\Gamma_3 \neq 0$ the density ρ decays algebraically to its asymptotic zero value. In one dimension the asymptotic time behavior is dominated by fluctuations and we expect that $\rho \sim t^{-1/2}$ instead of the mean field behavior $\rho \sim t^{-1}$.

The main purpose of the present work is to give, for the free fermion case, an exact solution of the reaction-diffusion problem. The formalism used here avoids the Wigner-Jordan transformation and exploits, instead, the quasiblock diagonal property of the evolution operator, obtained when using an appropriate representation, and the property, common to any stochastic process described by a master equation, that the *reference* vector (the leading left eigenvector of the evolution operator) is always known *a priori*. We use a representation in which the occupied and empty sites are associated to the spinors $\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $\begin{pmatrix} 1 \\ -1 \end{pmatrix}$, respectively, instead of the usual representation. In this representation, the evolution operator transforms a given vector into a vector with the same number of kinks or into a vector with two more kinks, which implies a quasiblock diagonal property to the evolution operator. The number of kinks in a generic vector will be defined below. Moreover, the reference state is a vector with no kinks.

The approach presented here allows us to easily recover the exact results obtained previously by other methods [1,5,10] and to get new ones such as the time dependent density profile corresponding to a traveling bump (or hollow). We find that, for large times, the bump, or the hollow, moves with a velocity $2(\Gamma_2 - \Gamma_1)$ so that the effect of driving can be absorbed by a Galilean transformation to a reference frame moving with such a velocity in accordance with a result of Schütz [9].

II. MODEL

We consider a reaction-diffusion one-species process occurring on a one-dimensional lattice of N sites described by a master equation. Each site is either empty or occupied by at most one particle. A configuration is represented by means of variables η_i , $i = 1, 2, \dots, N$, such that η_i takes the values 0

or 1 according to whether the site i is empty or occupied. The time evolution of the probability distribution $P(\eta, t)$ of a configuration $\eta = (\eta_1, \eta_2, \dots, \eta_N)$ at time t is governed by the master equation

$$\frac{d}{dt}P(\eta, t) = \sum_i \{w(1 - \eta_i, 1 - \eta_{i+1})P(\eta^{i,i+1}, t) - w(\eta_i, \eta_{i+1})P(\eta, t)\}, \quad (1)$$

where $\eta^{i,i+1}$ stands for $(\eta_1, \dots, 1 - \eta_i, 1 - \eta_{i+1}, \dots, \eta_N)$ and $w(\eta_i, \eta_j)$ is the transition rate, given by $w(00) = \Gamma_0$, $w(01) = \Gamma_1$, $w(10) = \Gamma_2$, and $w(11) = \Gamma_3$. Periodic boundary conditions are used, that is, $\eta_{N+1} = \eta_1$.

Next we wish to represent the probability of a configuration as a vector in a convenient vector space. To this end we attach to each site i a ket vector $|\sigma_i\rangle$ that may be either the column matrix $\binom{1}{0} \equiv |+\rangle$ or $\binom{0}{1} \equiv |-\rangle$. The whole vector space is then represented by the ket basis vectors $|\sigma\rangle \equiv |\sigma_1 \sigma_2 \dots \sigma_N\rangle = |\sigma_1\rangle \otimes |\sigma_2\rangle \otimes \dots \otimes |\sigma_N\rangle$, a direct product of the vectors $|\sigma_i\rangle$. Similarly one introduces the row matrices $(1 \ 0) \equiv \langle +|$ and $(1 \ 1) \equiv \langle -|$, and the bra basis vectors $\langle \sigma|$. A given configuration of particles η is associated to the ket vector $|\eta\rangle \equiv |\eta_1\rangle \otimes |\eta_2\rangle \otimes \dots \otimes |\eta_N\rangle$ where $|\eta_i\rangle$ is either $\binom{1}{1} \equiv |1\rangle = |+\rangle + |-\rangle$ or $\binom{1}{-1} \equiv |0\rangle = |+\rangle - |-\rangle$ according to whether $\eta_i = 1$ (occupied site) or $\eta_i = 0$ (empty site), respectively. At time t the state of the system is then represented by the vector $|\Psi(t)\rangle$ defined by

$$|\Psi(t)\rangle = \sum_{\eta} P(\eta, t) |\eta\rangle. \quad (2)$$

Analogously, one defines the bra vector $\langle \eta| = \langle \eta_1| \otimes \langle \eta_2| \otimes \dots \otimes \langle \eta_N|$ where $\langle \eta_i|$ can be either the vector $\langle 1| \equiv \frac{1}{2}(\langle +| + \langle -|)$ or $\langle 0| \equiv \frac{1}{2}(\langle +| - \langle -|)$. The reference vector $\langle O| = \sum_{\eta} \langle \eta| = \langle + + + \dots +|$ plays a special role in the present formalism because besides being a leading eigenvector of the evolution operator it gives the sum of the coefficients of the expansion in $\langle \eta|$ of any ket vector. In particular, the density of particles ρ_i at site i is $\rho_i = \langle O| \hat{n}_i |\Psi(t)\rangle$, where \hat{n}_i is the number operator at site i , defined by $\hat{n}_i |1\rangle = |1\rangle$ and $\hat{n}_i |0\rangle = 0$ so that $\hat{n}_i |\pm\rangle = (|\pm\rangle + |-\rangle)/2$.

The reaction-diffusion process considered here conserves parity, that is, if one starts with a configuration with an even (odd) number of particles, the system will always stay with an even (odd) number of particles. This means that the evolution operator splits into two nonconnecting sectors: an even and an odd sector. For simplicity we will restrict ourselves to the even sector and consider the number of sites N to be even.

By inspection we see that

$$P_{\pm}(\eta) = \prod_i (\pm p)^{\eta_i} (1-p)^{1-\eta_i} \quad (3)$$

are stationary solutions of the master equation (1), where the parameter $p = \sqrt{\Gamma_0}/(\sqrt{\Gamma_0} + \sqrt{\Gamma_3})$. These solutions are independent of the diffusion parameters Γ_1 and Γ_2 and are valid

as long as Γ_1 and Γ_2 are not both zero. The stationary state $|\Psi_{\text{ev}}\rangle$ belonging to the even sector is set up then as a linear combination of these solutions, namely,

$$|\Psi_{\text{ev}}\rangle = \frac{1}{1 + (2p-1)^N} \sum_{\eta} \{P_+(\eta) + P_-(\eta)\} |\eta\rangle, \quad (4)$$

from which one obtains the stationary density of particles

$$\rho_s = p \frac{1 + (2p-1)^{N-1}}{1 + (2p-1)^N}, \quad (5)$$

which in the limit $N \rightarrow \infty$ gives the result $\rho_s = p$.

The time evolution equation

$$\frac{d}{dt} |\Psi(t)\rangle = W |\Psi(t)\rangle \quad (6)$$

of the state vector is obtained from the master equation (1) by using standard techniques [3,4,18]. The evolution operator $W = \sum_i W_{i,i+1}$ is a sum of operators such that $W_{i,i+1}$ acts locally on the neighboring sites i and $i+1$ and has the matrix representation

$$W_{i,i+1} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ a & c & d & b \\ b & d & c & a \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (7)$$

where

$$a = \frac{1}{2}(-\Gamma_3 + \Gamma_2 - \Gamma_1 + \Gamma_0), \quad (8)$$

$$b = \frac{1}{2}(-\Gamma_3 - \Gamma_2 + \Gamma_1 + \Gamma_0), \quad (9)$$

$$c = \frac{1}{2}(-\Gamma_3 - \Gamma_2 - \Gamma_1 - \Gamma_0), \quad (10)$$

$$d = \frac{1}{2}(-\Gamma_3 + \Gamma_2 + \Gamma_1 - \Gamma_0). \quad (11)$$

From now on we restrict ourselves to the case $\Gamma_0 + \Gamma_3 = \Gamma_2 + \Gamma_1$. In this case the elements $\langle + - | W_{i,i+1} | - + \rangle = d$ and $\langle - + | W_{i,i+1} | + - \rangle = d$ vanish and the evolution operator W acquires a remarkable property. Let us define the number of kinks in the vector $|\sigma\rangle$ as the number of $+ -$ and $- +$ pairs in the configuration $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_N)$. For example, the vector $|+ + + - - + +\rangle$ has two kinks. The action of W on a right vector $|\sigma\rangle$ with n kinks gives either right vectors with n kinks or right vectors with $n+2$ kinks. Equivalently, the action of W on a left vector $\langle \sigma|$ with n kinks gives either left vectors with n kinks or left vectors with $n-2$ kinks.

Denote by P_n the operator that projects out states with n kinks; this property can be written as $P_n W P_{n'} = 0$ unless $n' = n$ or $n' = n - 2$. From this it follows that

$$W = \sum_n P_n W P_n + \sum_n P_n W P_{n-2} \quad (12)$$

so that the matrix W splits into blocks, each one of them connecting subspaces with a definite number of kinks. The nonvanishing blocks are those belonging to the diagonal ($n' = n$) and to the left subdiagonal ($n' = n - 2$). All blocks to the right of the diagonal vanish, implying that the eigenvalues of the W are the same as those of the block diagonal matrix

$$\tilde{W} = \sum_n P_n W P_n. \quad (13)$$

The eigenvectors of \tilde{W} can then be classified according to the number of kinks they have. We denote by $|\tilde{\Psi}_{nk}\rangle$ and $\langle\tilde{\Psi}_{nk}|$ the right and left normalized eigenvectors of \tilde{W} belonging to the sector of n kinks and by Λ_{nk} the associated eigenvalue. The corresponding eigenvectors of W , denoted by $|\Psi_{nk}\rangle$ and $\langle\Psi_{nk}|$, do not possess, in general, a definite number of kinks. However, they have the following structure:

$$|\Psi_{nk}\rangle = |\tilde{\Psi}_{nk}\rangle + |\zeta_{n+2,k}\rangle + |\zeta_{n+4,k}\rangle + \dots, \quad (14)$$

$$\langle\Psi_{nk}| = \langle\tilde{\Psi}_{nk}| + \langle\zeta_{n-2,k}| + \langle\zeta_{n-4,k}| + \dots, \quad (15)$$

where $|\zeta_{nk}\rangle$ and $\langle\zeta_{nk}|$ denote general vectors belonging to the sector of n kinks. In particular, the left and right eigenvectors corresponding to $n=0$ are $\langle O_{\text{ev}}| = (\langle +++ \dots | + \langle --- \dots |)/2$ and the stationary state $|\Psi_{\text{ev}}\rangle$ given by Eq. (4). Since $\langle O_{\text{ev}}|$ is the only left vector belonging to the sector of zero kink, the left eigenvector $\langle\Psi_{2,k}|$ corresponding to $n=2$ must be, according to Eq. (15), a linear combination of $\langle\tilde{\Psi}_{2,k}|$ and $\langle O_{\text{ev}}|$. Imposing the orthogonality with the right eigenvector $|\Psi_{\text{ev}}\rangle$ we get

$$\langle\Psi_{2,k}| = \langle\tilde{\Psi}_{2,k}| - \langle\tilde{\Psi}_{2,k}|\Psi_{\text{ev}}\rangle\langle O_{\text{ev}}|. \quad (16)$$

The time evolution of the state vector is given by the formal solution of Eq. (6), that is, by $|\Psi(t)\rangle = e^{tW}|\Psi(0)\rangle$ from which we obtain

$$|\Psi(t)\rangle = |\Psi_{\text{ev}}\rangle + \sum_{n(\neq 0),k} e^{t\Lambda_{nk}} |\Psi_{nk}\rangle \langle\Psi_{nk}|\Psi(0)\rangle. \quad (17)$$

From this expression it follows that

$$\begin{aligned} \rho_i = \rho_s + \frac{1}{2} \sum_k e^{t\Lambda_{2,k}} \langle O|\sigma_i^x|\tilde{\Psi}_{2,k}\rangle \\ \times \{ \langle\tilde{\Psi}_{2,k}|\Psi(0)\rangle - \langle\tilde{\Psi}_{2,k}|\Psi_{\text{ev}}\rangle \}, \end{aligned} \quad (18)$$

where we have taken into account that $\hat{n}_i = (1 + \sigma_i^x)/2$ and that $\langle O|\sigma_i^x$ is a vector belonging to the sector with two kinks. We used also the results (14), (15), (16), the orthogonality between vectors with distinct number of kinks, and the normalization $\langle O_{\text{ev}}|\Psi(0)\rangle = 1$. The calculation of the density profile by the relation (18) is then reduced to the determination of the eigenvectors of \tilde{W} within the sector of two kinks.

III. DENSITY PROFILE

Eigenvectors of \tilde{W} with two kinks are obtained as follows. First, let us introduce the notation

$$|\phi_{\ell/m}\rangle = \begin{cases} |1 \quad \ell \quad m \quad N\rangle \\ |++++--++\rangle, & \ell < m \quad (19) \\ |1 \quad m \quad \ell \quad N\rangle \\ |----+++-\rangle, & m < \ell. \quad (20) \end{cases}$$

These vectors form a closed subspace of vectors with two kinks and the eigenvalue equation $\tilde{W}|\phi_{\ell/m}\rangle = \Lambda|\phi_{\ell/m}\rangle$ is

$$\begin{aligned} 2c|\phi_{\ell/m}\rangle + a|\phi_{\ell-1,m}\rangle + a|\phi_{\ell,m-1}\rangle \\ + b|\phi_{\ell+1,m}\rangle + b|\phi_{\ell,m+1}\rangle = \Lambda|\phi_{\ell/m}\rangle \end{aligned} \quad (21)$$

and is valid for $\ell \neq m$. Such an eigenvalue problem is similar to the problem of two spin waves in the Heisenberg ferromagnet [27] and is better treated by introducing sum and difference coordinates [27]. We define then new coordinates u and v by $u = (\ell + m)/2$ and $v = (m - \ell)/2$ when $1 \leq \ell < m \leq N$ and $u = \text{mod}((\ell + m + N)/2, N)$ and $v = (m - \ell + N)/2$ when $1 \leq m < \ell \leq N$. The solution of the eigenvalue equation gives the right eigenvectors

$$|\tilde{\Psi}_{KQ}\rangle = \sum_{uv} e^{-iKu} \sin Qv |\Phi_{uv}\rangle, \quad (22)$$

where $|\Phi_{uv}\rangle = |\phi_{\ell/m}\rangle$ and the possible values of K and Q are $K = 2\pi n_1/N$ and $Q = 2\pi n_2/N$ with $n_1, n_2 = 0, 1, \dots, N-1$. The corresponding eigenvalues are

$$\Lambda_{KQ} = 2c + 2(ae^{-iK/2} + be^{iK/2}) \cos \frac{Q}{2}. \quad (23)$$

Similarly we obtain the normalized left eigenvectors

$$\langle\tilde{\Psi}_{KQ}| = \frac{2}{N^2} \sum_{uv} \langle\Phi_{uv}| e^{iKu} \sin Qv. \quad (24)$$

The density of particles at a given site m is given by

$$\rho_m = \rho_s + \frac{1}{2} \sum_{KQ} e^{t\Lambda_{KQ}} \langle \Phi_{m-1/2,1/2} | \tilde{\Psi}_{KQ} \rangle \times \{ \langle \tilde{\Psi}_{KQ} | \Psi(0) \rangle - \langle \tilde{\Psi}_{KQ} | \Psi_{ev} \rangle \}. \quad (25)$$

A straightforward calculation gives

$$\langle \tilde{\Psi}_{KQ} | \Psi_{ev} \rangle = -\frac{1}{N} \delta_{K,0} \frac{\sin Q/2}{A + \cos Q/2} (1 - e^{iQN/2}), \quad (26)$$

where $A = c/(a+b)$ and

$$\langle \Phi_{m-1/2,1/2} | \tilde{\Psi}_{KQ} \rangle = e^{-iK(m-1/2)} \sin \frac{Q}{2}. \quad (27)$$

We consider initial states that are uncorrelated, that is, states such that the probability distribution is of the Bernoulli type. Actually we will consider as the initial state the projection of such a state over the even sector, given by

$$|\Psi(0)\rangle = \frac{1}{Z} \sum_{\eta} I(\eta) \prod_i (\rho_i)^{\eta_i} (1 - \rho_i)^{1 - \eta_i} |\eta\rangle, \quad (28)$$

where $I(\eta) = 1 + \prod_i (-1)^{\eta_i}$ and $Z = 1 + \prod_i (2\rho_i - 1)$ is the normalization constant.

First, we will treat the case of a translational invariant initial state, that is, such that $\rho_i = \rho_0$ independent of the site. In this case a straightforward calculation gives

$$\langle \tilde{\Psi}_{KQ} | \Psi(0) \rangle = \frac{2}{N} \delta_{K,0} \frac{\sin Q/2}{B - \cos Q/2} (1 - e^{iQN/2}), \quad (29)$$

where $B = [(2\rho_0 - 1)^{-1} + 2\rho_0 - 1]/2$. Substituting this expression and expressions (26) and (27) in Eq. (25) and after taking the limit $N \rightarrow \infty$ we obtain the time dependent density

$$\rho = \rho_s + \frac{1}{4\pi} \int_0^{2\pi} e^{t\Lambda_{0,Q}} \frac{(A+B)\sin^2 Q/2}{(A + \cos Q/2)(B - \cos Q/2)} dQ, \quad (30)$$

which is independent of the site.

When $\Gamma_0 = 0$, $A = 1$ and this expression reduces to the one obtained by Santos *et al.* [10]. For the case $\rho_0 = 1$, a lattice initially full of particles, $B = 1$, and expression (30) gives a result obtained by Grynberg *et al.* [5]. If, moreover, $\Gamma_0 = 0$ we have $\rho_s = 0$, $A = B = 1$ so that

$$\rho = \frac{1}{\pi} \int_0^\pi e^{-2t\Gamma_3(1 - \cos \theta)} d\theta = e^{-2t\Gamma_3} I_0(2t\Gamma_3), \quad (31)$$

where $I_0(z)$ is the Bessel function of zero order. This result was obtained by Lushnikov [1] and also by Grynberg *et al.* [5]. The asymptotic behavior of the density for large times is $\rho \sim (4\pi t\Gamma_3)^{-1/2}$.

We consider finally the case of an initial density profile displaying a bump (or a hollow). The initial state is uncorre-

lated and the density at any site is $\rho_i = 1/2$ except the site $i = N/2$ for which the density is $\rho_{N/2} = \rho_a$. A straightforward calculation gives

$$\langle \tilde{\Psi}_{KQ} | \Psi(0) \rangle = \frac{2}{N^2} (2\rho_a - 1) (e^{iKN/2} - e^{iQN/2}) e^{-iK/2} \sin \frac{Q}{2}. \quad (32)$$

Substituting this expression and expressions (26) and (27) in Eq. (25) and making the translation $\ell = m - N/2$ we obtain, after taking the limit $N \rightarrow \infty$, the time dependent density profile

$$\rho_{\ell} = \rho_c + \frac{(2\rho_a - 1)}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} e^{t\Lambda_{KQ}} e^{-iK\ell} \sin^2 \frac{Q}{2} dK dQ, \quad (33)$$

where ρ_c is a site independent term which coincides with the right hand side of Eq. (30) for the density corresponding to an initial homogeneous condition $\rho_i = 1/2$.

Expression (33) gives the exact density profile at any time. To find the long time behavior one expands the integrand in small K and Q . The result is

$$\rho_{\ell} = \rho_c + \frac{(2\rho_a - 1)}{2\pi(2t|\Gamma_3 - \Gamma_0|)^2} \times \exp\left(-\frac{[\ell - 2t(\Gamma_2 - \Gamma_1)]^2}{4t|\Gamma_3 - \Gamma_0|} - 4t\Gamma\right), \quad (34)$$

where $\Gamma = \Gamma_0$ if $\Gamma_3 > \Gamma_0$ and $\Gamma = \Gamma_3$ if $\Gamma_3 < \Gamma_0$. The density profile exhibits a Gaussian bump, if $\rho_a > 1/2$, or a hollow, if $\rho_a < 1/2$. For large times the bump, or the hollow, moves with a velocity $2(\Gamma_2 - \Gamma_1)$ so that the effect of driving can be absorbed by a Galilean transformation to a reference frame moving with such a velocity in accordance with a result of Schütz [9]. The horizontal size of the bump, or hollow, increases as $[4t|\Gamma_3 - \Gamma_0|]^{1/2}$ whereas its vertical size decreases as $t^{-2} e^{-4t\Gamma}$.

IV. CONCLUSION

We have provided a derivation of the exact density profile of a one-dimensional reaction-diffusion process where hardcore particles, subject to diffusion, can be annihilated and created. The solution is possible because, in the representation used here and within the free fermion condition, the evolution operator W transforms vectors with a certain number of kinks into vectors with the same number of kinks or with two more kinks. This property implies that W has the same set of eigenvalues as the block diagonal operator \tilde{W} . The calculation of the density profile is reduced to the determination of the eigenvectors of \tilde{W} within the sector of two kinks. The calculation of the two-site correlations is also possible but needs the eigenvectors belonging to the sector of four kinks. Our approach allows us to recover exact results already known and to obtain new ones such as the time dependent density profile of a traveling bump.

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