Diffusion-limited reactions of hard-core particles in one dimension

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We investigate three different methods to tackle the problem of diffusion-limited reactions (annihilation) of hard-core classical particles in one dimension. We first extend an approach devised by Lushnikov [Sov. Phys. JETP **64**, 811 (1986)] and calculate for a single species the asymptotic long-time and/or large-distance behavior of the two-point correlation function. Based on a work by Grynberg and Stinchcombe [Phys. Rev. E **50**, 957 (1994); Phys. Rev. Lett. **74**, 1242 (1995); **76**, 851 (1996)], which was developed to treat stochastic adsorption-desorption models, we provide in a second step the exact two-point (one- and two-time) correlation functions of Lushnikov's model. We then propose a formulation of the problem in terms of path integrals for pseudofermions. This formalism can be used to advantage in the multispecies case, especially when applying perturbative renormalization group techniques. [S1063-651X(99)03902-1]

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I. INTRODUCTION

The recent interest in modeling low-dimensional diffusion-limited reactions has been stimulated in part by the experimental observation of anomalous kinetics in low-dimensional systems [1]. The traditional approach to chemical reactions is based on mean-field theory, i.e., rate equations for the densities of the various reactants. The latter describe well the reaction kinetics in three dimensions because diffusive transport of reactants allows one to eliminate the spatial fluctuations of the concentrations. However, in lower dimensions, due to the lack of phase space, the reactants spatial fluctuations can grow and develop inhomogeneities in the concentrations. Furthermore, even in the spatially homogeneous case, the rate equations are not applicable in less than three dimensions; for example, in the two-species diffusion-limited annihilation the concentration of the particles decays (for identical initial concentrations) slower than the mean-field theory predicts. Thus the fluctuation-dominated dynamics is beyond the classical theories, yet can be accounted for by simple one-dimensional (1D) models of hard-core particles. The latter are solved either numerically or analytically by applying techniques from (classical or quantum) statistical mechanics [1]. In particular, exact solutions have been obtained by interparticle distribution methods by relating the systems to dual and solvable 1D models [2–5] (kinetic Ising and Potts) and by mapping the diffusion-reaction processes to an imaginary-time dynamics of quantum spin chains with non-Hermitian Hamiltonians [5]. An alternative and fruitful approach has been developed by Cardy and collaborators [6–9]: The idea is to reformulate the original problem in terms of a field theory of interacting bosons and subsequently use renormalization group techniques. This is a powerful method as it applies to arbitrary dimension and low densities of particles, a regime where universal behavior (scaling) is usually observed. Despite the progress achieved in this field, the multispecies case is still poorly understood. Furthermore, when the density of particles is high, the hard-core constraint on the dynamics of the diffusing particles becomes important. Experimentally, the single-species fusion model used to describe the photoluminescence of excitons diffusing along one-dimensional chains is seen to apply only as long as the initial exciton densities are small [1]. To our knowledge, there has been no systematic effort yet to investigate theoretically the regime of high densities of reactants.

This is a technical paper in which we will explore an approach that attempts to remedy the difficulties encountered so far. We propose to start from a quantum spin chain formulation of the master equation, fermionize (introduce a basis of fermion states), and subsequently apply renormalization group techniques to deal with the interaction terms arising in the multispecies case. Note that in the single species case, the method applies at arbitrary densities as the hard core of the classical particles is automatically accounted for by the Fermi statistics. When various species react and diffuse, it is appropriate to distinguish two cases. (i) The various species have infinite on-site repulsion with themselves only; this can be treated readily following the methods outlined in the following sections. (ii) The particles of different species all have a hard-core constraint; this is far more difficult and will be investigated elsewhere. As with the other methods devised so far, there is a price to pay: The calculations involved are sometimes extremely tedious.

The purpose of this paper is modest as we will focus on the single-species case for which fermion-fermion interactions do not arise as a consequence of mapping classical particles to fermions. We want to show explicitly how by elementary means we can reproduce known results (the long-time behavior of the density) and derive some other results, i.e., the explicit and exact analytical form of the two-point correlation one- and two-time functions. The paper is intended as an introduction to the fermionic functional integration approach that we plan to combine in future work with the renormalization techniques to treat the multispecies case.

In Sec. II we define the model, introduce notation, and review an extension of a method developed by Lushnikov. Section III is devoted to the application of an elegant technique introduced by Grynberg and Stinchcombe in a different context to evaluate the two-point (one-time) correlation function. Section IV deals with a powerful formulation of the problem in terms of path integrals of pseudofermionic variables. We illustrate the technique by computing the two-time correlation function. A brief discussion concludes the paper in Sec. V.

II. LUSHNIKOV'S APPROACH

This section introduces notation and summarizes and extends Lushnikov's genuine approach. We consider a lattice of N (even) sites (length $L=Na$, $a=1$, and assume $N/2$ even), with periodic boundary conditions, on which classical (spinless) particles with a hard core can diffuse (annihilate) to adjacent empty (occupied) sites with rate D. Whenever the arrival site is occupied, an annihilation reaction $(1+1\to\emptyset)$ takes place. A source of intensity J injects pairs of particles on adjacent sites $(\emptyset\to 1+1)$. Lushnikov [10] has managed to rewrite the master equation that describes the annihilation and diffusion processes described above in terms of an imaginary-time Schrödinger equation

$$\frac{d}{dt}|\psi(t)\rangle=\mathcal{L}|\psi(t)\rangle, \qquad (1)$$

where $\mathcal{L}$ denotes the so-called Liouvillian, which by abuse of language we will call a non-Hermitian Hamiltonian. $|\psi(t)\rangle$ represents the state of the system at time t,

$$|\psi(t)\rangle=\sum_{\{n\}}\left(P(\{n\},t)\prod_{m'(\{n\})}\sigma^{+}_{m'(\{n\})}\right)|0\rangle, \qquad (2)$$

where $m'(\{n\})$ represents the sites of configuration $\{n\}$ that are occupied. The Liouvillian is given by [10]

$$\mathcal{L}=(J+D)\sum_m(\sigma_m^+\sigma_{m+1}^+ +\sigma_m^+\sigma_{m+1}^- +\sigma_m^-\sigma_{m+1}^+ +\sigma_m^-\sigma_{m-1}^-)$$
$$+D\sum_m(\sigma_{m+1}^-\sigma_m^- -\sigma_{m+1}^+\sigma_m^+ -2\sigma_m^+\sigma_m^-)-JN. \qquad (3)$$

When $J=0$, i.e., there is no source, in addition to diffusive processes with a rate D, only irreversible reactions $(1+1\to\emptyset)$ with rate $2D$ take place.

For a finite $(J>0)$ source, the diffusive processes $(1+\emptyset\to\emptyset+1$ and $\emptyset+1\to 1+\emptyset)$ take place with rate $J+D$ and we also have reversible reactions: Particles are annihilated $(1+1\to\emptyset)$ with rate $J+2D$ and created $(\emptyset\to 1+1)$ with rate J. It is worth emphasizing that these rates are not independent and are chosen such that the Liouvillian is quadratic in the spin variables for a single species (the higher-order terms cancel due to the properties of Pauli matrices). In the n-species case, this property no longer holds if we assume hard-core repulsion between all species. Indeed, one obtains a spin Hamiltonian $(S=n/2)$ that is a polynomial of higher order in the spin operators and in general cannot be solved exactly. If, however, we assume infinite on-site repulsion only between particles of the same species, we can rewrite the Hamiltonian as a quadratic form of coupled spins 1/2. The latter can be solved by the techniques presented below. We also point out that in this model the ''annihilation rate'' $(J+2D)$ is always bigger than the ''creation rate'' (J).

To solve the Schrödinger equation in imaginary time, Lushnikov performs a Jordan-Wigner transformation and introduces the fermionic operators $a_m=\prod_{j<m}(1-2n_j)\sigma_m^-$. Because of the form of the resulting non-Hermitian Hamiltonian, it is appropriate to work with Fourier modes $a_q=(e^{i(\pi/4)}/\sqrt{N})\sum_m a_m e^{-iqm}$. The antiperiodic boundary conditions [11] lead to $q=\pm(2l-1)\pi/N$, $l=1,2,\ldots,N/2$. On Fourier transforming, the evolution operator reads $\mathcal{L}=\sum_{q>0}\mathcal{L}_q$, where $(n_q\equiv a_q^+a_q)$

$$\mathcal{L}_q=2(J+D)[\cos q(n_q+n_{-q})+\sin q(a_q a_{-q}-a_q^\dagger a_{-q}^\dagger)]$$
$$+2D[\sin q(a_q a_{-q}+a_q^\dagger a_{-q}^\dagger)-(n_q+n_{-q})]-JN. \qquad (4)$$

Now, by a BCS-like ansatz

$$|\psi(t)\rangle=\prod_{q>0}|\psi_q(t)\rangle=\prod_{q>0}[A_q(t)a_q^\dagger a_{-q}^\dagger+B_q(t)]|0\rangle, \qquad (5)$$

Lushnikov [10] is able to decouple the dynamical equation as

$$\frac{d}{dt}|\psi_q(t)\rangle=\mathcal{L}_q|\psi_q(t)\rangle \quad \forall \quad q>0. \qquad (6)$$

For a lattice that is initially completely occupied, i.e., $A_q(0)=1$ and $B_q(0)=0$, one solves the above equations using

$$A_q(t)=\frac{1}{4(J+2D)\sin^2\left(\frac{q}{2}\right)}(p_2e^{p_2t}-p_1e^{p_1t}),$$

$$B_q(t)=\frac{-(J+2D)\sin q}{2(J+2D)\sin^2\left(\frac{q}{2}\right)}(e^{p_2t}-e^{p_1t}), \qquad (7)$$

where

$$p_1=-2(J+2D)(1-\cos q), \quad p_2=2J(1+\cos q). \qquad (8)$$

In the absence of a source $(J=0)$, the solution simplifies considerably to

$$A_q(t)=\exp[-4Dt(1-\cos q)],$$

$$B_q(t)=\cot\left(\frac{q}{2}\right)\{\exp[-4Dt(1-\cos q)-1]\}. \qquad (9)$$

At this point it is worth noting that the ket $|\psi(t)\rangle$ characterizes the state of the system at any time without, however, being an eigenvector of $\mathcal{L}$ (the Liouvillian is not normal; however, see below).

In Ref. [10] Lushnikov calculates the density of particles by the method of the generating function, which we extend in order to evaluate the two-point correlation function. The density reads

$$\rho(t)=\sum_{\{n\}} \tilde{n}_i(\{n\})P(\{n\},t) \quad \forall \;\; i, \tag{10}$$

where $\tilde{n}_i=0,1$ is the eigenvalue of the occupation operator $n_i=a_i^\dagger a_i$. Similarly, the two-point correlation function is written as

$$\mathcal{G}_r(t)\equiv\langle \tilde{n}_i\tilde{n}_{i+r}\rangle(t)=\sum_{\{n\}} \tilde{n}_i(\{n\})\tilde{n}_{i+r}(\{n\})P(\{n\},t), \tag{11}$$

where the translational symmetry of the system has been used. We observe that in this formalism

$$\rho(t)=\langle 0|\exp\left(\sum_n \sigma_n^-\right)n_i|\psi(t)\rangle,$$

$$\mathcal{G}_r(t)=\langle 0|\exp\left(\sum_n \sigma_n^-\right)n_i n_{i+r}|\psi(t)\rangle, \tag{12}$$

as one can check using the explicit form of $|\psi(t)\rangle$ (develop the exponential, order each term, and perform a Jordan-Wigner transformation [10]). It is appropriate to consider the generating function

$$G(x,y,z,t)=\langle 0|\exp\left(x\sigma_i^- + y\sigma_{i+r}^- + z\sum_{n\neq i,i+r}\sigma_n^-\right)|\psi(t)\rangle$$
$$=\sum_{\{n\}} x^{\tilde{n}_i}y^{\tilde{n}_{i+r}}z^{\Sigma_j\tilde{n}_j-\tilde{n}_i-\tilde{n}_{i+r}}P(\{n\},t). \tag{13}$$

So we have

$$\rho(t)=\frac{\partial}{\partial x}G(x,z,z,t)\Big|_{x,y,z=1},$$

$$\mathcal{G}_r(t)=\frac{\partial^2}{\partial x\,\partial y}G(x,y,z,t)\Big|_{x,y,z=1}. \tag{14}$$

To compute the generating function, we rewrite the state as

$$|\psi(t)\rangle=\prod_{q>0}[A_q(t)a_q^\dagger a_{-q}^\dagger + B_q(t)]|0\rangle$$
$$=\prod_{q>0}\left(B_q(t)-\frac{2A_q(t)}{N}\sum_{n>m}a_m^\dagger a_n^\dagger \sin(q[n-m])\right)|0\rangle. \tag{15}$$

Note the normalization condition due to the conservation of probability

$$\sum_{\{n\}} P(\{n\},t)=\prod_{q>0}\left(B_q(t)-A_q(t)\cot\frac{q}{2}\right)=1. \tag{16}$$

Next expand the argument of the exponential as

$$G(x,y,z,t)$$
$$=\langle 0|\Bigg\{ \mathbb{1}+(xa_i+ya_{i+r}+z)$$
$$\times\sum_{n\neq i,i+r}a_n+\Bigg[z^2\sum_{i+r\neq n>n'\neq i}a_n a_{n'}$$
$$+xz\left(a_i\sum_{n<i}a_n+\sum_{n>i,n\neq i+r}a_n a_i\right)$$
$$+yz\left(\sum_{n>i+r}a_n a_{i+r}+a_{i+r}\sum_{n<i+r,n\neq i}a_n\right)$$
$$+xya_{i+r}a_i\Bigg]+\cdots\Bigg\}\prod_{q>0}$$
$$\times\left(2\frac{A_q(t)}{N}\sum_{n>m}a_m^\dagger a_n^\dagger \sin(q[n-m])-B_q(t)\right)|0\rangle. \tag{17}$$

In this expression, only the terms proportional to "xy" contribute to $\mathcal{G}_r(t)$. Let us call the first of these terms G_1,

$$G_1=\langle 0|xya_{i+r}a_i$$
$$\times\sum_{q>0}\Bigg\{2\frac{A_q(t)}{N}\sum_{n>m}a_m^\dagger a_n^\dagger\frac{\sin(q[n-m])}{A_q(t)\cot\frac{q}{2}-B_q(t)}$$
$$\times\prod_{q\neq q'>0}\left(\frac{B_{q'}(t)}{B_{q'}(t)-A_{q'}(t)\cot\frac{q'}{2}}\right)\Bigg\}|0\rangle$$
$$=xy\frac{2}{N}\left(\sum_{q>0}\frac{\sin qr}{\cot\frac{q}{2}-\frac{B_q(t)}{A_q(t)}}\right)\left(\prod_{q\neq q'>0}\frac{1}{1-\frac{A_{q'}(t)}{B_{q'}(t)}\cot\frac{q}{2}}\right). \tag{18}$$

In the absence of source, we have $A_q(t)\to 0$ and $B_q(t)\to -\cot(q/2)$ exponentially fast [see Eq. (9)], so that in the thermodynamic limit ($N\to\infty$), the asymptotic behavior of $\mathcal{G}_r(t)$ follows as

$$\mathcal{G}_r(t)\sim\frac{\partial^2}{\partial x\,\partial y}G_1\to\frac{1}{\pi}\int_0^\pi\frac{dq\,\sin qr}{\cot\frac{q}{2}-\frac{B_q(t)}{A_q(t)}}. \tag{19}$$

We can do the same for the density and in the thermodynamic limit one obtains

$$\rho(t)=\frac{\partial}{\partial x}\prod_{q>0}\langle 0|\Bigg\{\mathbb{1}+\Bigg(xa_i+z\sum_{n\neq i}a_n\Bigg)$$
$$+\Bigg[z^2\sum_{i\neq n,n',n>n'}a_na_{n'}$$
$$+xz\Bigg(a_i\sum_{n<i}a_n+\sum_{n>i}a_na_i\Bigg)+\cdots\Bigg]\Bigg\}$$
$$\times\Bigg(2\frac{A_q(t)}{N}\sum_{n>m}a_m^\dagger a_n^\dagger\sin(q[n-m])$$
$$-B_q(t)\Bigg)|0\rangle\Bigg|_{z=1,\,x=0}$$
$$\to\frac{1}{\pi}\int_0^\pi\frac{dq}{1-\dfrac{B_q(t)}{A_q(t)\cot\frac{q}{2}}}. \tag{20}$$

In the above, we used the identities

$$\sum_{m>i}\sin(q[m-i])=\frac{1}{2}\left(\cot\frac{q}{2}+\frac{\cos(q[i-\frac{1}{2}])}{\sin\frac{q}{2}}\right),$$
$$\sum_{m<i}\sin(q[m-i])=\frac{1}{2}\left(\cot\frac{q}{2}-\frac{\cos(q[i-\frac{1}{2}])}{\sin\frac{q}{2}}\right)$$
$$\Rightarrow\sum_{n>m}\sin(q[n-m])=\frac{N}{2}\cot\frac{q}{2}. \tag{21}$$

The evaluation of the two-point correlation function requires the calculation of all the terms proportional to xy, which in general is a very hard task. In the following sections we will be able to solve this difficulty by reformulating the problem in a different language.

Using the explicit form of $A_q(t)$ and $B_q(t)$ [Eqs. (7)–(9)] and the results of the Appendix, we find the asymptotic behavior of the density in the (*irreversible*) *critical case* as [10]

$$\rho(t)=\frac{e^{-4Dt}}{\pi}\int_0^\pi dq\,e^{4Dt\cos q}=e^{-4Dt}I_0(4Dt)\sim\frac{1}{\sqrt{8\pi Dt}}. \tag{22}$$

Similarly, the asymptotic behavior of the two-point correlation function is

$$\mathcal{G}_r(t)\sim\frac{e^{-4Dt}}{\pi}\int_0^\pi dq\,\frac{\sin qr}{\sin q}(1-\cos q)e^{4Dt\cos q}$$
$$=e^{-4Dt}\sum_{0\leqslant n<r}[I_{2n-r+1}(4Dt)-I_{2n-r}(4Dt)]$$
$$\sim\frac{\pi r}{(8\pi Dt)^{3/2}}, \tag{23}$$

which implies for the connected correlation function that

$$C_r(t)\equiv G_r(t)-\rho^7(t)\sim-\frac{1}{8\pi Dt}. \tag{24}$$

Unfortunately, in the massive case (when the source intensity is finite), this method applies only to the computation of the density. Assuming $Dt,Jt\gg 1$, we find that

$$\rho(t)=\rho_{eq}+2(J+2D)$$
$$\times\int_t^\infty dt'\,e^{-4(J+D)t'}[I_0(4Dt')-I_1(4Dt')] \tag{25}$$
$$\sim\frac{\sqrt{J}}{\sqrt{J}+\sqrt{J+2D}}+\left(1+\frac{J}{2D}\right)\frac{e^{-4Jt}}{8Jt\sqrt{8\pi Dt}}, \tag{26}$$

where $\rho_{eq}=\sqrt{J}/(\sqrt{J}+\sqrt{J+2D})$ represents the equilibrium value of the density, in agreement with Lushnikov's result [10]. In the next section we provide the full two-point correlation function for $J>0$.

III. THE PSEUDOFERMIONIC APPROACH

In this section we evaluate the full two-point correlation function in the general case by means of a powerful formalism. The central idea is to perform on the fermionic non-Hermitian (and non-normal) Hamiltonian a generalized Bogoliubov transformation, which allows us to work with a diagonal evolution operator (see Refs. [12,13]). Following previous works [12–14,5], we denote each of the 2^N possible configurations by a ket $|n\rangle$:

$$\langle n|n'\rangle=\delta_{n,n'},\quad\sum_n|n\rangle\langle n|=\mathbb{1}. \tag{27}$$

In this Fock space, we can efficiently record the probabilities for the various configurations in the ket

$$|P(t)\rangle\equiv\sum_n P(n,t)|n\rangle. \tag{28}$$

The master equation governing the dynamics of the annihilation and diffusion processes described in Sec. II can be rewritten as

$$\frac{\partial}{\partial t}|P(t)\rangle=\mathcal{U}|P(t)\rangle=\sum_n\partial_tP(n,t)|n\rangle$$
$$=\sum_{n,n'}[A(n'\to n)P(n',t)-A(n\to n')P(n,t)]|n\rangle, \tag{29}$$

where $\mathcal{U}$ denotes the evolution operator and $A(n'\to n)$ and $A(n\to n')$ represent the transition rates expressed in terms of J and D in Lushnikov's formulation. The matrix elements for the operator $\mathcal{U}$ are

$$\langle n'|\mathcal{U}|n\rangle=A(n\to n')\quad\forall\ n'\neq n, \tag{30}$$

$$\langle n|\mathcal{U}|n\rangle = -\sum_{n'\neq n} A(n\to n'). \tag{31}$$

This Fock-space formulation was used in Refs. [12,13] to study a stochastic adsorption-desorption problem. In what follows we will specifically focus on the reaction-diffusion problem in one dimension.

Let us now introduce the left and right steady states, respectively,

$$\langle\tilde{\chi}| \equiv \sum_n \langle n|, \quad |\chi\rangle \equiv \sum_n P(n,\mathrm{eq})|n\rangle, \tag{32}$$

where $P(n,\mathrm{eq})$ denotes the probability for a configuration $|n\rangle$ at equilibrium. It is easy to check that $e^{\mathcal{L}t}$ has no effect on $|\chi\rangle$ and $\langle\tilde{\chi}|$ and the conservation of probability leads to $\langle\tilde{\chi}|\chi\rangle = 1$. The transition probability from a configuration $|n\rangle$ to $|n'\rangle$ is simply $W_{n,n'}(t) \equiv \langle n'|e^{\mathcal{L}t}|n\rangle$.

We intend to calculate the density and two-point one-time correlation functions of a system initially in the state $|\phi_0\rangle \equiv \Sigma_n P(n,t=0)|n\rangle$. The occupation number operator n_r being diagonal in the basis $\{|n\rangle\}$, we have

$$\rho(t) = \sum_{n,n'} \langle n'|n_r|n'\rangle W_{n,n'}(t) P(n,t=0)$$
$$= \sum_{n,n'} \langle n'|n_r e^{\mathcal{L}t}|n\rangle P(n,t=0) = \langle\tilde{\chi}|n_r e^{\mathcal{L}t}|\phi_0\rangle \tag{33}$$

and similarly

$$\mathcal{G}_r(t) = \sum_{n,n'} \langle n'|n_l n_m|n'\rangle W_{n,n'}(t) P(n,t=0)$$
$$= \sum_{n,n'} \langle n'|n_l n_m e^{\mathcal{L}t}|n\rangle P(n,t=0) = \langle\tilde{\chi}|n_l n_m e^{\mathcal{L}t}|\phi_0\rangle, \tag{34}$$

where $r = |m-l|$. At this point, we perform a generalized Bogoliubov transformation (rotation supplemented by a rescaling)

$$\begin{pmatrix} \xi_q^\dagger \\ \xi_{-q} \end{pmatrix} = \begin{pmatrix} \alpha\cos\theta_q & \alpha^{-1}\sin\theta_q \\ -\alpha\sin\theta_q & \alpha^{-1}\cos\theta_q \end{pmatrix} \begin{pmatrix} a_q^\dagger \\ a_{-q} \end{pmatrix} \tag{35}$$

in order to obtain a diagonal representation for the evolution operator. This transformation is orthogonal, i.e., invertible and canonical, in the sense that it preserves the anticommutation relations of the a_q's, namely,

$$\{\xi_q^\dagger, \xi_{q'}\} = \delta_{q,q'}, \quad \{\xi_q^\dagger, \xi_{q'}^\dagger\} = \{\xi_q, \xi_{q'}\} = 0. \tag{36}$$

Despite the fact that the ξ_q and $\xi_q^\dagger$ *are not adjoint* of each other, this representation will be very useful in the following. We set $\alpha = [J/(J+2D)]^{1/4}$, so that the mode q evolution operator becomes

$$-\mathcal{L}_q = 2[D(1-\cos q) - J][(\xi_q^\dagger\xi_q + \xi_{-q}^\dagger\xi_{-q})\cos^2\theta_q$$
$$+(\sin^2\theta_q)(\xi_{-q}\xi_{-q}^\dagger + \xi_q\xi_q^\dagger) + 2(\xi_{-q}^\dagger\xi_q^\dagger + \xi_q\xi_{-q})]$$
$$+\sqrt{J(J+2D)}\sin q[(\cos 2\theta_q)(\xi_{-q}^\dagger\xi_q^\dagger + \xi_q\xi_{-q})$$
$$+(\sin 2\theta_q)(\xi_q\xi_q^\dagger + \xi_{-q}^\dagger\xi_{-q})] + 2J. \tag{37}$$

To get rid of the terms that do not conserve the number of pseudoparticles we choose θ_q as

$$\tan 2\theta_q = \frac{\sqrt{J(J+2D)}\sin q}{(J+D)\cos q - D} \tag{38}$$

so that the Hamilton operator becomes

$$\mathcal{L} = -\sum_{q>0} \lambda_q(\xi_q^\dagger\xi_q + \xi_{-q}^\dagger\xi_{-q}) = -\sum_q \lambda_q \xi_q^\dagger\xi_q, \tag{39}$$

where

$$\lambda_q = 2[D(1-\cos q) + J] \tag{40}$$

on account of the periodic boundary conditions ($\Sigma_{q>0}\cos q = 0$). Now it is readily seen that $\langle\tilde{\chi}|$ and $|\chi\rangle$ act, respectively, as left and right vacua, i.e., $\xi_q|\chi\rangle = 0$ and $\langle\tilde{\chi}|\xi_q^\dagger = 0$. To simplify the calculations, we express the initial ket state $|\phi_0\rangle$ in terms of the steady state $|\chi\rangle$. We consider here two kinds of initial conditions. (i) The whole lattice is initially filled. We write $|\phi_0\rangle = |\mathrm{all}\rangle$ and immediately conclude $a_q^\dagger|\mathrm{all}\rangle = 0$. Using the inverse of Eq. (35), one can check that

$$|\mathrm{all}\rangle = \prod_{q>0} [1 - (\cot\theta_q)\xi_q^\dagger\xi_{-q}^\dagger]|\chi\rangle$$
$$= \exp\left(-\sum_q \frac{\cot\theta_q}{2}\xi_q^\dagger\xi_{-q}^\dagger\right)|\chi\rangle. \tag{41}$$

(ii) The lattice is initially empty. One can check in the same way [14] that

$$|\phi_0\rangle = |0\rangle = \prod_{q>0}[1 + (\tan\theta_q)\xi_q^\dagger\xi_{-q}^\dagger]|\chi\rangle$$
$$= \exp\left(\sum_q \frac{\tan\theta_q}{2}\xi_q^\dagger\xi_{-q}^\dagger\right)|\chi\rangle. \tag{42}$$

The time dependences of $\xi_k(t)$ and $\xi_k^\dagger(t)$ follow as

$$\xi_k(t) = e^{-\mathcal{L}t}\xi_q e^{\mathcal{L}t} = e^{-\lambda_q t}\xi_k, \tag{43}$$

$$\xi_k^\dagger(t) = e^{-\mathcal{L}t}\xi_q^\dagger e^{\mathcal{L}t} = e^{\lambda_q t}\xi_k^\dagger. \tag{44}$$

Futhermore, we have

$$\langle\xi_{k_1}\xi_{k_2}\rangle(t=0) \equiv \langle\tilde{\chi}|\xi_{k_1}\xi_{k_2}|\mathrm{all}\rangle = (\cot\theta_{k_1})\delta_{k_1,-k_2} \tag{45}$$

and

$$\langle \xi_{k_1}\xi_{k_2}\xi_{k_3}\xi_{k_4}\rangle(t=0) = (\cot\theta_{k_1})(\cot\theta_{k_3})\delta_{k_1,-k_2}\delta_{k_3,-k_4} + (\cot\theta_{k_1})(\cot\theta_{k_2})(\delta_{k_1,-k_4}\delta_{k_2,-k_3} - \delta_{k_1,-k_3}\delta_{k_2,-k_4}), \tag{46}$$

as one can check by applying Wick's theorem (see also Sec. IV). Using the properties of the Fourier transform and the generalized Bogoliubov transformation (35), the expression of the density and the two-point correlation function become, respectively (for a lattice initially filled, $|\phi_0\rangle=|\text{all}\rangle$),

$$\rho(t)=\frac{1}{N}\sum_k \sin^2\theta_k - \sum_{k,k'}\frac{e^{i(k'-k)l}}{N}\sin\theta_k\cos\theta_{k'}\langle\tilde{\chi}|\xi_{-k}\xi_{k'}e^{\mathcal{L}t}|\text{all}\rangle \tag{47}$$

and one can do the same for unconnected one-time correlation function $\mathcal{G}_r(t)$ [Eq. (34)].

To derive tractable formulas, we have performed tedious but straightforward calculations. Indeed, we have extracted the time dependence of $\rho(t)$ and $\mathcal{G}_r(t)$ using Eq. (43) and commuted all the pseudocreation operators to the left of the pseudoannihilation operators. In the expression of $\rho(t)$ and $\mathcal{G}_r(t)$ only terms such as $\langle\tilde{\chi}|\xi_{-k}\xi_{k'}|\text{all}\rangle=\langle\xi_{-k}\xi_{k'}\rangle\ (t=0)$ and $\langle\tilde{\chi}|\xi_{-k}\xi_{k'}\xi_{-q}\xi_{q'}|\text{all}\rangle=\langle\xi_{-k}\xi_{k'}\xi_{-q}\xi_{q'}\rangle\ (t=0)$ survive: These were evaluated with the help of Eqs. (45) and (46). In the thermodynamic limit, we arrive at

$$\begin{aligned}\rho(t)&=\frac{2}{N}\sum_{k>0}(\sin^2\theta_k+e^{-2\lambda_k t}\sin\theta_k\cos\theta_k\cot\theta_k)\\ &\to\frac{1}{\pi}\int_0^\pi dq(\sin^2\theta_q+e^{-2\lambda_q t}\cos^2\theta_q)\\ &=\frac{\sqrt{J}}{\sqrt{J}+\sqrt{J+2D}}+2(J+2D)\\ &\quad\times\int_t^\infty dt'[I_0(4Dt')-I_1(4Dt')]e^{-4(J+D)t'},\end{aligned} \tag{48}$$

which coincides with Eq. (25).

It is worth emphasizing that this result is general and works for both the *massive* $(J\neq 0)$ and the *critical* $(J=0)$ cases. The point here is that the limit $J\to 0$ is not singular, despite the divergence of $\cot\theta\to-\infty$. In fact, integration over k and k' of terms proportional to $\sin\theta_k\cot\theta_{k'}$ yields finite results. Therefore, we can perform the computations (35) at J finite and set subsequently $J=0$ in $\rho(t)$ and $\mathcal{G}_r(t)$.

Similarly, the two-point (one-time) correlation function is evaluated for a lattice initially filled as $(r=|m-l|)$

$$\mathcal{G}_r(\text{eq})=\rho_{eq}^2+\frac{1}{\pi^2}\left(\int_0^\pi dq\sin^2\theta_q\cos qr\right)\left(\int_0^\pi dq'\cos^2\theta_{q'}\cos q'r\right)+\left(\frac{1}{2\pi}\int_0^\pi dq\sin 2\theta_q\sin qr\right)^2, \tag{49}$$

$$\begin{aligned}\mathcal{G}_r(t)-\mathcal{G}_r(\text{eq})=&[\rho(t)^2-\rho_{\text{eq}}^2]+\frac{1}{\pi^2}\left(\int_0^\pi dq\,e^{-2\lambda_q t}\cos^2\theta_q\cos qr\right)\left(\int_0^\pi dq'\cos^2\theta_{q'}\cos q'r\right)\\ &+\frac{1}{2\pi^2}\left(\int_0^\pi dq\sin 2\theta_q\sin qr\right)\left(\int_0^\pi dq' e^{-2\lambda_{q'}t}\cos^2\theta_{q'}\cot\theta_{q'}\sin q'r\right)\\ &-\frac{1}{\pi^2}\left(\int_0^\pi dq\sin^2\theta_q\cos qr\right)\left(\int_0^\pi dq'\,e^{-2\lambda_{q'}t}\cos^2\theta_{q'}\cos q'r\right)\\ &-\frac{1}{4\pi^2}\left(\int_0^\pi dq\sin 2\theta_q\sin qr\right)\left(\int_0^\pi dq'\,e^{-2\lambda_{q'}t}\sin 2\theta_{q'}\sin q'r\right)-\left(\frac{1}{\pi}\int_0^\pi dq\,e^{-2\lambda_q t}\cos^2\theta_q\cos qr\right)^2\\ &-\left(\frac{1}{\pi^2}\int_0^\pi dq\,e^{-2\lambda_q t}\cos^2\theta_q\cot\theta_q\sin qr\right)\left(\int_0^\pi dq'\,e^{-2\lambda_{q'}t}\sin^2\theta_{q'}\cot\theta_{q'}\sin qr\right),\end{aligned} \tag{50}$$

where we separated the static contribution to the correlation function from the dynamic one. Using known properties of modified Bessel functions given (see the Appendix) and writing $I'_m(x)\equiv(d/dx)I_m(x)$, we finally infer [notice that $\mathcal{G}_r(\text{eq})=\rho_{\text{eq}}^2$]

$$\mathcal{G}_r(t)=\rho(t)^2+2(J+2D)(A_0-C_0)\int_t^\infty dt'\,e^{-4(J+D)t'}[I_r(4Dt')-I'_r(4Dt')]$$
$$+\frac{\sqrt{J(J+2D)}B_0}{2}\int_t^\infty dt'\,e^{-4(J+D)t'}\frac{r}{2Dt'}I_r(4Dt')$$
$$-\frac{(J+2D)^{3/2}}{\sqrt{J}}\sum_{0\leqslant n<r}\left(\int_t^\infty dt'\,e^{-4(J+D)t'}\{2I_{2n-r+1}(4Dt')-2I_{2n-r}(4Dt')+I'_{2n-r}(4Dt')\}\right)$$
$$-\left(2(J+2D)\int_t^\infty dt'\,e^{-4(J+D)t'}[I_r(4Dt')-I'_r(4Dt')]\right)^2$$
$$+2(J+2D)^2\left[\sum_{0\leqslant n<r}(2n-r)\left(\int_t^\infty dt'\,e^{-4(J+D)t'}\frac{I_{2n-r}(4Dt')}{2Dt'}\right)\right]$$
$$\times\left[\sum_{0\leqslant n<r}\left(\int_t^\infty dt'\,e^{-4(J+D)t'}\{2I_{2n-r+1}(4Dt')-2I_{2n-r}(4Dt')+I'_{2n-r}(4Dt')\}\right)\right]. \tag{51}$$

In the above formula A_0,B_0,C_0 have been defined by

$$A_0\equiv\frac{1}{\pi}\int_0^\pi dq\,\cos^2\theta_q\cos qr,\quad B_0\equiv\frac{1}{\pi}\int_0^\pi dq\,\sin 2\theta_q\sin qr,$$
$$C_0\equiv\frac{1}{\pi}\int_0^\pi dq\,\sin^2\theta_q\cos qr \tag{52}$$

or, more explicitly, in the massive case [with the help of Eq. (A12)],

$$A_0=\frac{J+2D}{\pi}\int_0^\pi\frac{dq}{\lambda_q}\left(\cos qr-\frac{\cos q(r+1)+\cos q(r-1)}{2}\right)$$
$$=-(J+2D)\zeta^{r-1}\frac{(1-\zeta)^2}{4\sqrt{J^2+2JD}}, \tag{53}$$

$$B_0=\frac{\sqrt{J(J+2D)}}{\pi}\int_0^\pi\frac{dq}{\lambda_q}[\cos q(r+1)-\cos q(r-1)]$$
$$=-\zeta^{r-1}\frac{1-\zeta^2}{2}, \tag{54}$$

$$C_0=\frac{J}{\pi}\int_0^\pi\frac{dq}{\lambda_q}\left(\cos qr+\frac{\cos q(r+1)+\cos q(r-1)}{2}\right)$$
$$=J\zeta^{r-1}\frac{(1+\zeta)^2}{4\sqrt{J^2+2JD}}, \tag{55}$$

with the notation

$$\zeta\equiv\frac{D}{(J+D)+\sqrt{J^2+2JD}}\leqslant 1. \tag{56}$$

The formula can be evaluated numerically. The connected two-point correlation function $\mathcal{C}_r(t)\equiv\mathcal{G}_r(t)-\rho(t)^2$ follows immediately from the above. To establish a connection with the results derived previously [5] we explicitly evaluate $\mathcal{C}_r(t)$ when $J=0$. Paying due attention to the apparent singularities occurring in this limit, we find

$$\mathcal{C}_r(t)=\frac{1}{2\pi^2}\int_0^\pi dq\,\sin 2\theta_q\sin qr$$
$$\times\int_0^\pi dq'\,e^{-2\lambda_{q'}t}\cot\theta_{q'}\sin q'r$$
$$-\left(\frac{1}{\pi}\int_0^\pi dq\,e^{-2\lambda_q t}\cos qr\right)^2$$
$$-\left(\frac{1}{\pi}\int_0^\pi dq\,e^{-2\lambda_q t}\cot\theta_q\sin qr\right)$$
$$\times\left(\frac{1}{\pi}\int_0^\pi dq'\,e^{-2\lambda_{q'}t}\sin^2\theta_{q'}\cot\theta_{q'}\sin qr\right) \tag{57}$$

or, in terms of elementary functions,

$$\mathcal{C}_r(t)=\sum_{0\leqslant n<r}e^{-4Dt}[I_{2n-r+1}(4Dt)-I_{2n-r}(4Dt)]$$
$$+\left(\sum_{0\leqslant n<r}e^{-4Dt}I_{2n-r}\right)^2$$
$$-\left(\sum_{0\leqslant n<r}e^{-4Dt}I_{2n-r+1}\right)^2-[e^{-4Dt}I_r(4Dt)]^2. \tag{58}$$

This expression is equivalent to the result derived by a well-known mapping of Lushnikov's model to Glauber's 1D Ising model [5].

Finally, we compute [using formula (A11)] the asymptotic behavior of the two-point correlation function $\mathcal{C}_r(t)$ for $Dt\gg 1$, $Jt\gg 1$, and $r<\infty$,

$$\mathcal{C}_r(t) \sim -\frac{\zeta^{r-1}e^{-4Jt}}{8Jt\sqrt{8\pi Dt}}\Bigg\{(J+2D)(1-\zeta)^2+J(1+\zeta)^2 + \frac{rJ(J+2D)}{D}(1-\zeta^2)\Bigg\}\frac{1}{4\sqrt{J(J+2D)}}. \tag{59}$$

As expected for a finite source intensity $J>0$, the density and one-time correlation function decay exponentially with time. Morever, the one-time correlation function also decays exponentially with distance.

A similar calculation can be performed for the case of an initial empty lattice ($|\phi_0\rangle \equiv |0\rangle$). In this case the density is $\rho(t)=2J\int_t^\infty dt'[I_0(4Dt')+I_1(4Dt')]e^{-4(J+D)t'} \sim \rho_{\rm eq} - e^{-4Jt}/\sqrt{8\pi Dt}$ [10]. It has been shown [12], via the mapping to the Glauber dynamics, that the nearest neighbor connected function decays ($Dt, Jt \gg 1$) as $\mathcal{C}_{r=1}^{(t)} \sim \rho_{eq}e^{-4Jt}/\sqrt{2\pi Dt}$.

The large-time and large-distance behavior of the one-time correlation function can also be studied. In fact, in the critical case it has been shown [4,5] that the one-time correlation function obeys a scaling form.

Here we investigate the behavior of $\mathcal{C}_r(t)$ in the limit where r and $Dt\to\infty$ with $u\equiv r^2/8Dt$ finite. In the massive case, we do not expect a scaling form

$$\mathcal{C}_r(t) \sim -\sqrt{1+\frac{2D}{J}}\zeta^{r-1}(1-\zeta^2)\frac{g(r^2,u)}{4r^2}, \tag{60}$$

where

$$g(r^2,u) \equiv \sqrt{\frac{u^3}{\pi}}e^{-Jr^2/2Du}. \tag{61}$$

The effect of the source is to disrupt the spatial correlations, i.e., to make them short ranged. In this sense the finite source prohibits the formation of arbitrarily large vacancy domains.

In the next section we will introduce a field-theoretic approach to deal with two-time correlation function. Our approach and the results obtained thereby complement the exact treatments of the critical case [15]. It is worth pointing out that Glauber calculated in his pioneering work the two-time two-point spin correlations functions [2,16].

IV. FIELD THEORETICAL REFORMULATION

The purpose of this section is to reformulate the results of the preceding section in field-theoretic language, i.e., in terms of path integrals of fermionic variables (see, for example, [17]). We define the Grassmann numbers η_q, η_q^*, which anticommute with each other and with the fermionic operators introduced in the preceding section, i.e., $\{\eta_q,\eta_{q'}\}=\{\eta_q^*,\eta_{q'}^*\}=\{\eta_q^*,\eta_{q'}\}=0$ and $\{\eta_q,\xi_{q'}\} = \{\eta_q^*,\xi_{q'}^\dagger\}=\{\eta_q^*,\xi_{q'}\}=\{\eta_q^*,\xi_{q'}^\dagger\}=0$. We follow standard practice and consider the *coherent states* associated with the fermionic variables. We recall that pseudofermionic operators requiring the introduction of a *left vacuum* $\langle\tilde{\chi}|$ and a *right vacuum* $|\chi\rangle$, ergo we define the right $|\eta\rangle$ and the left coherent states $\langle\tilde{\eta}|$, respectively, as $|\eta\rangle = \exp(-\Sigma_q\eta_q\xi_q^\dagger)|\chi\rangle$ and $\langle\tilde{\eta}| = \langle\chi|\exp(-\Sigma_q\xi_q\eta_q^*)$. Despite the fact that ξ and $\xi^\dagger$ are not adjoint of each other, we find the familiar results

$$\langle\tilde{\eta}|\chi\rangle = \langle\tilde{\chi}|\eta\rangle = 1,$$

$$\langle\tilde{\eta}|\eta\rangle = \exp\left(\sum_q \eta_q^*\eta_q\right), \quad \xi_q|\eta\rangle = \eta_q|\eta\rangle,$$

$$\langle\tilde{\eta}|\xi_q = \frac{\partial}{\partial\eta_q^*}\langle\tilde{\eta}|, \quad \langle\tilde{\eta}|\xi_q^\dagger = \langle\tilde{\eta}|\eta_q^*, \quad \xi_q^\dagger|\eta\rangle = -\frac{\partial}{\partial\eta_q}|\eta\rangle.$$

Most importantly, the closure relation holds true, i.e.,

$$\int\prod_q d\eta_q^*\, d\eta_q \exp\left(-\sum_q \eta_q^*\eta_q\right)|\eta\rangle\langle\tilde{\eta}| = \mathbb{1}. \tag{62}$$

At this point, we know from field theory how to calculate $\langle\tilde{\chi}|n_m e^{\mathcal{L}t}|\text{all}\rangle$ and $\langle\tilde{\chi}|n_m n_{m+r}e^{\mathcal{L}t}|\text{all}\rangle$ using the path-integral formalism. We discretize time in M infinitesimal intervals of width $\epsilon\equiv\lim_{M\to\infty}(t/M)$. $\mathcal{L}$ is normally ordered and the closure relation is inserted into the above formulas. We have for the density (for the lattice initially filled)

$$\rho(t) = \int\prod_{q,\alpha=1,\ldots,M} d\eta_{q,\alpha}^*\, d\eta_{q,\alpha} \times\exp\left(-\sum_{q,\alpha}\eta_{q,\alpha}^*\eta_{q,\alpha}\right)\langle\tilde{\chi}|n_m|\eta_M\rangle \times\langle\tilde{\eta}_M|e^{\mathcal{L}\epsilon_M}|\eta_{M-1}\rangle\cdots\langle\tilde{\eta}_2|e^{\mathcal{L}\epsilon_2}|\eta_1\rangle\langle\tilde{\eta}_1|e^{\mathcal{L}\epsilon_1}|\text{all}\rangle, \tag{63}$$

where

$$\lim_{M\to\infty}\langle\tilde{\eta}_1|e^{\mathcal{L}\epsilon_1}|\text{all}\rangle = \exp\left(-\frac{1}{2}\sum_q \cot\theta_q\,\eta_{q,1}^*\eta_{-q,1}^*\right), \tag{64}$$

$$\begin{aligned}\langle\tilde{\chi}|n_m|\eta_M\rangle &= \frac{1}{N}\left(\sum_k \sin^2\theta_k - \sum_{k,k'}\sin\theta_k\cos\theta_{k'}\langle\tilde{\chi}|\xi_{-k}\xi_{k'}|\eta_m\rangle\right)\\ &= \frac{1}{N}\left(\sum_k \sin^2\theta_k - \sum_{k,k'}(\sin\theta_k\cos\theta_{k'})\eta_{k,M}\eta_{k',M}\right).\end{aligned} \tag{65}$$

Taking the continuum limit [17], we arrive at

$$\rho(t)=\frac{1}{N}\int\prod_q d\eta_q^*(t)\,d\eta_q(t)\times\left(\sum_k\sin^2\theta_k-\sum_{k,k'}\sin\theta_k\cos\theta_{k'}\,\eta_q(t)\,\eta_{q'}(t)\right)\times\exp\left(-\sum_q\frac{\cot\theta_q}{2}\eta_q^*(0)\,\eta_{-q}^*(0)\right)e^{-S_0(\eta^*(t),\eta(t))},\tag{66}$$

where the Liouvillian operator $\mathcal{L}$ acts as the *Hamiltonian* of field theory. By abuse of language we call $S_0(\eta^*(t),\eta(t))$ the *Euclidean action* of our problem, which is defined by

$$S_0(\eta^*(t),\eta(t))\equiv\int_0^t dt'\sum_q[\eta_q^*(t')\partial_{t'}\eta_q(t')-\mathcal{L}(\eta_q^*(t'),\eta_q(t'))]+\sum_{q'}\eta_{q'}^*(0)\,\eta_{q'}(0).\tag{67}$$

Taking averages $\langle\,\rangle_{S_0}$ on the Gaussian distribution, the density can be rewritten as

$$\rho(t)=\frac{1}{N}\left\langle\left(\sum_k\sin^2\theta_k-\sum_{k,k'}(\sin\theta_k\cos\theta_{k'})\,\eta_q(t)\,\eta_{q'}(t)\right)\times\exp\left(-\sum_q\frac{\cot\theta_q}{2}\eta_q^*(0)\,\eta_{-q}^*(0)\right)\right\rangle_{S_0}.\tag{68}$$

We proceed to discretize the free Euclidean action S_0, which is bilinear, as

$$S(q)=\begin{pmatrix}1&0&0&\dots&\dots&0\\-a&1&0&\dots&\dots&0\\0&-a&1&0&\dots&0\\\vdots&\ddots&\ddots&\ddots&\vdots&\vdots\\0&\ddots&\ddots&\ddots&\vdots&0\\0&\dots&\dots&0&-a&1\end{pmatrix},\tag{69}$$

where $a\equiv1-(t/M)\lambda_q$.

Following Ref. [17], we find $\det[S(q)]=1$ and

$$\lim_{M\to\infty}S^{-1}_{\alpha,\beta}(q)=e^{-\lambda_q(t_\alpha-t_\beta)}\quad\forall\ \alpha=1,\dots,M\geqslant\beta,\quad t_\alpha=\frac{\alpha t}{M}.\tag{70}$$

Furthermore, we have in the continuum limit $[\int\prod_q d\eta_q^*(t)\,d\eta_q(t)e^{-S_0}=1]$

$$\langle\eta_p(t_2)\,\eta_{p'}^*(t_1)\rangle_{S_0}=\int\prod_q d\eta_q^*(t)\,d\eta_q(t)\,\eta_p(t_2)\,\eta_{p'}^*(t_1)e^{-S_0}=\delta_{p,p'}e^{-\lambda_p(t_2-t_1)}.\tag{71}$$

Applying Wick's theorem leads to

$$\langle\xi_p\xi_{p'}\rangle(t)=\left\langle\eta_p(t)\,\eta_{p'}(t)\times\exp\left(-\frac{1}{2}\sum_q(\cot\theta_q)\,\eta_q^*(0)\,\eta_{-q}^*(0)\right)\right\rangle_{S_0}=\delta_{p,-p'}(\cot\theta_p)e^{-2\lambda_p t}.\tag{72}$$

With this result, it is straightforward to calculate the density using Eqs. (72) and (68).

The computation of the correlation function requires evaluation of terms such as $\langle\xi_{k1}\xi_{k2}\xi_{k3}\xi_{k4}\rangle(t)$. We generate in the standard fashion the multipoint correlation functions. The generating functional in discretized time reads

$$Z[g_{q,\alpha};g^*_{q',\alpha'}]=\left\langle\exp\left(\sum_q\left\{-\frac{1}{2}(\cot\theta_q)\,\eta^*_{q,1}\eta^*_{-q,1}+\sum_{\alpha\geqslant2}(g^*_{q,\alpha}\eta_{q,\alpha}+\eta^*_{q,\alpha}g_{q,\alpha})\right\}\right)\right\rangle_{S_0}.\tag{73}$$

Here $g_{q,\alpha},g^*_{q,\alpha}$ (Grassman numbers) denote the coefficient of the source terms. Note that this functional differs from the usual field-theoretic one [17] by a term that codes the initial condition, i.e., $\prod_{q>0}e^{\cot\theta_q\eta^*_{q,1}\eta^*_{-q,1}}$. Taking this term into account, however, is no trouble, i.e.,

$$Z[g_{q,\alpha};g^*_{q',\alpha'}]=\left\{\prod_{q>0}(e^{g^*_{-q,1}g^*_{q,1}\cot\theta_q}+g^*_{-q,1}g^*_{q,1}g_{-q,1}g_{q,1})\right\}\times\prod_{q,q'}\prod_{i,j=2}^{M}e^{g^*_{q,i}S_{i,j}(q)^{-1}g_{q',j}\delta_{q,q'}}.\tag{74}$$

Considering that the source term will be set to zero in the end of the calculation and noting that for $\alpha=1$ only pseudo-creation operators contribute, we find it convenient to work with

$$\tilde{Z}[g_{q,\alpha};g^*_{q',\alpha'}]=\prod_q \exp\left(\frac{1}{2}g^*_{-q,1}g^*_{q,1}\cot\theta_q + \sum_{q'}\sum_{i,j>1} g^*_{q,i}e^{\lambda_q(t_j-t_i)}g_{q',j}\delta_{q,q'}\right). \quad (75)$$

From the definition it follows then that

$$\langle \xi_{k_1}\xi_{k_2}\rangle(t)=\left.\frac{\delta^6\tilde{Z}[g_{q,\alpha};g^*_{q',\alpha'}]}{\delta g_{-q,1}\delta g^*_{q,1}\delta g^*_{k_1,M}\delta g^*_{k_2,M}\delta g_{q,2}\delta g_{-q,2}}\right|_{g=g^*=0} \quad (76)$$

or, more generally,

$$\langle \xi_{k_1}\xi_{k'_1}\cdots\xi_{k_n}\xi_{k'_n}\rangle(t) \equiv\langle\tilde{\chi}|\xi_{k_1}\xi_{k'_1}\cdots\xi_{k_n}\xi_{k'_n}e^{\mathcal{L}t}|\text{all}\rangle=\langle\tilde{\chi}|\xi_{k_1}\xi_{k'_1}\cdots\xi_{k_n}\xi_{k'_n}e^{\mathcal{L}t}\exp\left(-\frac{1}{2}\sum_q \cot\theta_q\xi^\dagger_q\xi^\dagger_{-q}\right)|\chi\rangle$$
$$=\left.\frac{\delta^{6n}\tilde{Z}[g_{q,\alpha};g^*_{q',\alpha'}]}{\delta g^*_{-q_n,1}\delta g^*_{q_n,1}\cdots\delta g^*_{-q_1,1}\delta g^*_{q_1,1}\delta g^*_{k_1,M}\delta g^*_{k'_1,M}\cdots\delta g^*_{k_n,M}\delta g^*_{k'_n,M}\delta g_{q_1,2}\delta g_{-q_1,2}\cdots\delta g_{q_n,2}\delta g^*_{-q_n,2}}\right|_{g=g^*=0}. \quad (77)$$

As an application of this field-theoretic formulation we will now extend our approach to the computation of the two-time correlation function for an initial state $|\phi_0\rangle$,

$$\mathcal{G}_r(t,t')\equiv\langle n_{l+r}(t+t')n_l(t)\rangle=\langle\tilde{\chi}|n_l e^{\mathcal{L}t'}n_{l+r}e^{\mathcal{L}t}|\phi_0\rangle$$
$$=\sum_{n,n'}\langle n'|n_{l+r}e^{\mathcal{L}t'}n_l e^{\mathcal{L}t}|n\rangle P(n,0)$$
$$=\sum_{n,n',n''}\langle n'|n_{l+r}|n'\rangle\langle n''|n_l|n''\rangle W_{n'n''}(t')W_{n''n}(t)P(n,0). \quad (78)$$

As above, we consider an initially filled lattice ($|\phi_0\rangle=|\text{all}\rangle$).

To perform the computation of $\mathcal{G}(r,t,t')$ we need to evaluate terms such as

$$\langle\tilde{\chi}|\xi_p\xi_{p'}e^{\mathcal{L}t'}\xi_q\xi_{q'}e^{\mathcal{L}t}|\text{all}\rangle=\left\langle \eta_p(t+t')\,\eta_{p'}(t+t')\,\eta_q(t)\,\eta_{q'}(t)\exp\left(-\frac{1}{2}\sum_k \cot\theta_k\,\eta^*_k(0)\,\eta^*_{-k}(0)\right)\right\rangle_{S_0}. \quad (79)$$

This expression can be calculated by using the generating functional, where as before t (t') is discretized into $M(N)$ infinitesimal time steps (respectively), with $M,N\to\infty$:

$$\langle\tilde{\chi}|\xi_p\xi_{p'}e^{\mathcal{L}t'}\xi_q\xi_{q'}e^{\mathcal{L}t}|\text{all}\rangle$$
$$=\left.\frac{\delta^{12}\tilde{Z}[g_{q,\alpha};g^*_{q',\alpha'}]}{\delta g^*_{-q_2,1}\delta g^*_{q_2,1}\delta g^*_{-q_1,1}\delta g^*_{q_1,1}\delta g^*_{q,M}\delta g^*_{q',M}\delta g^*_{p,M+N}\delta g^*_{p',M+N}\delta g_{q_1,2}\delta g_{-q_1,2}\delta g_{q_2,2}\delta g_{-q_2,2}}\right|_{g=g^*=0}$$
$$=e^{-(\lambda_p+\lambda_{p'})(t+t')-(\lambda_q+\lambda_{q'})t}[(\cot\theta_p\cot\theta_q\,\delta_{p,-p'}\delta_{q,-q'}+\cot\theta_p\cot\theta_{p'}\,(\delta_{-p,q'}\delta_{-q,p'}-\delta_{-q,p}\delta_{-p',q'})], \quad (80)$$

where the continuum limit for the time has been taken. Applying the same technique to each term of $\mathcal{G}(r,t,t')$ yields

$$
\begin{aligned}
\mathcal{G}_r(t,t') = {}& \rho_{\rm eq}^2 + 2(J+2D)\rho_{\rm eq}\int_t^\infty dT\, e^{-4(J+D)T}[I_0(4DT)-I_1(4DT)] \\
&+ J(J+2D)\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}[I_r(2DT)+I_r'(2DT)]\right)\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}[I_r(2DT)-I_r'(2DT)]\right) \\
&+ \frac{J(J+2D)}{4}\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}\frac{r}{DT}I_r(2DT)\right)^2 - 2(J+2D)^2\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}[I_r(2DT)-I_r'(2DT)]\right) \\
&\times\left(\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[I_r(2D(2T+t'))-I_r'(2D(2T+t'))]\right) \\
&+ (J+2D)^2\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}\frac{r}{2D(2T+t')}I_r(2DT)\right) \\
&\times\left(\sum_{0\leqslant n<r}\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[2I_{2n-r+1}(2D(2T+t'))-2I_{2n-r}(2D(2T+t'))+I_{2n-r}'(2D(2T+t'))]\right) \\
&+ J(J+2D)\left(\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[I_0(2D(2T+t'))-I_1(2D(2T+t'))]\right) \\
&\times\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}[I_0(2DT)+I_1(2DT)]\right) \\
&- \frac{J(J+2D)}{2}\left(\int_t^\infty dT\, e^{-2(J+D)(2T+t')}\frac{r}{D(2T+t')}I_r(2D(2T+t'))\right) \\
&\times\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}\frac{r}{DT}I_r(2DT)\right) - 2J(J+2D)\left(\int_{t'}^\infty dT\, e^{-2(J+D)T}[I_r(2DT)+I_r'(2DT)]\right) \\
&\times\left(\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[I_r(2D(2T+t'))-I_r'(2D(2T+t'))]\right) \\
&+ 4(J+2D)^2\left(\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[I_0(2D(2T+t'))-I_1(2D(2T+t'))]\right)^2 \\
&- 2(J+2D)^2\left(\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[I_r(2D(2T+t'))-I_r'(2D(2T+t'))]\right)^2 \\
&+ 2(J+2D)^2\left(\sum_{0\leqslant n<r}(2n-r)\int_t^\infty dT\, e^{-2(J+D)(2T+t')}\frac{I_{2n-r}(2D(2T+t'))}{D(2T+t')}\right) \\
&\times\left(\sum_{0\leqslant n<r}\int_t^\infty dT\, e^{-2(J+D)(2T+t')}[2I_{2n-r+1}(2D(2T+t'))-2I_{2n-r}(2D(2T+t'))+I_{2n-r}'(2D(2T+t'))]\right).
\end{aligned} \tag{81}
$$

In the critical case some care is required when taking $J\to 0$,

$$
\begin{aligned}
\mathcal{G}_r(t,t') = {}& e^{-4D(2t+t')}\{[I_0(2D(2t+t'))]^2 \\
&- [I_r(2D(2t+t'))]^2\} + De^{-2D(2t+t')}\left\{\int_{t'}^\infty dT\, e^{-2DT}\frac{r}{DT}I_r(2DT)\right\}\left\{\sum_{0\leqslant n<r}[I_{2n-r+1}(2D(2t+t')) \right. \\
&\left. - I_{2n-r}(2D(2t+t'))]\right\} + e^{-4D(2t+t')}\left\{\left(\sum_{0\leqslant n<r}I_{2n-r}(2D(2t+t'))\right)^2 - \left(\sum_{0\leqslant n<r}I_{2n-r+1}(2D(2t+t'))\right)^2\right\}.
\end{aligned} \tag{82}
$$

To study the behavior at finite distance of the two-time correlation function $\mathcal{C}_r(t,t')\equiv\mathcal{G}_r(t,t')-\rho(t)\rho(t')$ we distinguish the massive and the critical regimes. We begin with the massive case and consider $Dt,Dt'\gg 1; Jt,Jt'\gg 1$; and $r<\infty$. With the help of Eqs. (A8)–(A11) we have

$$\mathcal{G}_r(t,t')\sim\rho_{\rm eq}^2+\left(1+\frac{J}{2D}\right)\rho_{\rm eq}\frac{e^{-4Jt}}{8Jt\sqrt{8\pi Dt}},$$

$$\mathcal{C}_r(t,t')\sim-\left(1+\frac{J}{2D}\right)\rho_{eq}\frac{e^{-4Jt'}}{8Jt'\sqrt{8\pi Dt'}}. \tag{83}$$

When $r<\infty$, Dt and Jt are finite and $Dt',Jt'\gg 1$. We obtain

$$\mathcal{G}_r(t,t')\sim\rho_{\rm eq}^2+\frac{J+2D}{128J}\frac{e^{-4Jt'}}{(Dt')^2}$$
$$+\frac{J+2D}{4JD}\frac{e^{-4J(t+t')}}{16\pi D\sqrt{t'}(2t+t')^{3/2}},$$

$$\mathcal{C}_r(t,t')\sim-\left(1+\frac{J}{2D}\right)\rho_{\rm eq}\frac{e^{-4Jt'}}{8Jt'\sqrt{8\pi Dt'}}. \tag{84}$$

In the critical case $(r<\infty)$, both the asymptotic behavior $Dt,Dt'\gg 1$ and Dt finite with $Dt'\gg 1$ of the disconnected and connected correlation functions are given by

$$\mathcal{G}_r(t,t')\sim\frac{r^2}{4\pi D^2(2t+t')^2}\left(1+\frac{1}{8}\sqrt{1+\frac{2t}{t'}}\right),$$

$$\mathcal{C}_r(t,t')\sim-\frac{1}{8\pi D\sqrt{tt'}}. \tag{85}$$

Near the initial state (the density of particles is high), when $Dt,Dt'\ll 1$, the decay is linear and independent of r, i.e.,

$$\mathcal{G}_r(t,t')\sim 1-4D(2t+t'),$$

$$\mathcal{C}_r(t,t')\sim-4Dt. \tag{86}$$

We now provide a scaling form for the two-time correlation function $\mathcal{C}_r(t,t')$. It is known, from the duality with Glauber's model, that the single-time correlation function obeys a scaling form for large time and long distances (Dt and $r\to\infty$ with the ratio r^2/Dt held finite [4,5]). The scaling form is found as $\mathcal{C}_r(t)\sim r^{-2}f(r^2/4Dt)$, where the exponent -2 is believed to be universal [5]. We further assume the long-time and large-distance scaling form $\mathcal{C}_r(t,t')\sim r^{-y}h(u,v)$, where $r,Dt,Dt'\to\infty$ with $u\equiv r^2/4Dt$ and $v\equiv r^2/4Dt'$ held finite, and arrive at

$$\mathcal{C}_r(t,t')\sim\frac{1}{\pi r^2}\Bigg\{K^{3/2}e^{-K}(\sqrt{\pi}\mathrm{erf}\sqrt{v}-2\sqrt{K})$$
$$+K(1-e^{-2K})-\frac{\sqrt{uv}}{2}\Bigg\}, \tag{87}$$

where $0<K\equiv uv/(u+2v)<\infty$.

At this point it is appropriate to review what we have achieved so far. We have been able to reformulate the problem of the evaluation of the multipoint correlation functions in a language that parallels the field-theoretic one. This allows us to compute in an efficient and systematic way physical quantities of interest despite some technical differences from the standard approach. While this paper deals with a free "field theory" of pseudofermions, it is tempting to apply the same formalism to the multispecies case where two- or multibody interactions arise. The latter, however, will be investigated in a future work by pertubative renormalization group techniques, as no exact solutions are available.

V. CONCLUDING REMARKS

We have studied three different approaches to the problem of diffusion and annihilation of classical hard-core particles moving on a one-dimensional ring. Though Lushnikov's contributions to the problem are genuine and indisputable, we have shown how an extension of his generating function method to evaluate the two-point correlation function can be cumbersome in practice, even in the simplest case available of a single species. We have seen that it is advantageous to apply a generalized Bogoliubov transformation used by Grynberg and Stinchcombe [12,13] in a different context. The evolution operator can be diagonalized, i.e., expressed as a quadratic form of two operators that are not adjoint of each other. Despite this fact the formalism resembles the standard one and appears as a powerful tool. Indeed, we were able to compute the full one-time and two-time correlation functions for an initially fully occupied lattice (other initial conditions can also be studied) in the presence of a finite source. We derived a scaling form for the two-time correlation function. We used the results of Secs. II and III (algebraic decay in the critical case and exponential in the presence of a source) to check the asymptotic behavior of the density and two-point correlation function. We discovered that while in the absence of source the modes at long wavelengths fully control the long-time asymptotics of the density and correlation functions, in the presence of a finite source all modes contribute. This means that in the general case, the long-wavelength approximations that were so successful in strongly correlated systems (such as bosonization or conformal field theory techniques) do not work for the problem at hand. Moreover, the idea of exploiting the integrability of some spin Hamiltonians on which the multispecies Liouvillian maps might turn out to be more elusive than expected. In view of the above remark, it would seem extremely difficult if not impossible to extract from the exact Bethe-ansatz solution of the non-Hermitian spin Hamiltonian the relevant matrix elements that in turn allow the evaluation of correlation functions [5]. We propose to tackle the multispecies problem in terms of fermion functionals, the main difficulties arising from the two- and/or multibody interactions occurring in the process of mapping classical particles to fermions. We plan to illustrate the power of the formalism in another paper, where we plan to apply the renormalization group scheme. Besides the obvious advantage of formulating the problem in a field-theoretic language (perturbation theory, etc.), the method is applicable to arbitrary densities of particles and thus complements the approach developed by Cardy and collaborators [6–9]. In higher dimensions, however, Fermi statistics requires the introduction of a gauge field that is strongly coupled to the fermions. We also intend to explore this line of research in the future.

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APPENDIX: USEFUL RESULTS

In this appendix we provide some useful properties of the Bessel functions of imaginary argument. We recall the definition of the modified Bessel $I_n(z)$ function (n integer) [18]

$$I_n(z)=\frac{(-i)^n}{2\pi}\int_{-\pi}^{\pi}e^{z\sin(p)+inp}\,dp=\frac{1}{\pi}\int_0^{\pi}e^{z\cos\theta}\cos(n\theta)d\theta, \tag{A1}$$

with $I_n(z)=I_{-n}(z)$. We also use in Eqs. (51), (81), and (82) the well-known properties $I_{n-1}(z)-I_{n+1}(z)=(2n/z)I_n(z)$ and $I_{n-1}(z)+I_{n+1}(z)=2(d/dz)I_n(z)$. The following integrals occur in the evaluation of the two-point correlation function:

$$\tilde{I}_1(r,t)\equiv\int_0^{\pi}\frac{\sin qr}{\sin q}e^{4Dt\cos q}\,dq,$$

$$\tilde{I}_2(r,t)\equiv\int_0^{\pi}\frac{\sin qr}{\sin q}\cos q\,e^{4Dt\cos q}\,dq,$$

$$\tilde{I}_3(r,t)\equiv\int_0^{\pi}\frac{\sin qr}{\sin q}\cos 2q\,e^{4Dt\cos q}\,dq. \tag{A2}$$

Setting $\tilde{q}=q-i\epsilon$, with ϵ real and $\epsilon>0$, we have

$$\frac{\sin qr}{\sin q}=\lim_{\epsilon\searrow 0}\frac{\sin\tilde{q}r}{\sin\tilde{q}}, \tag{A3}$$

$$\begin{aligned}\frac{\sin qr}{\sin q}&=\lim_{\epsilon\searrow 0,q,\tilde{q}\to q}\frac{\sin\tilde{q}r}{\sin\tilde{q}}\\&=\lim_{\epsilon\searrow 0,\tilde{q}\to q}\sum_{n\geqslant 0}(e^{-2i\tilde{q}\{n-[(r-1)/2]\}}\\&\quad-e^{-2i\tilde{q}\{n+[(r+1)/2]\}}).\end{aligned} \tag{A4}$$

Therefore,

$$\begin{aligned}\tilde{I}_1(r,t)&=\int_0^{\pi}\left(\lim_{\epsilon\searrow 0,\tilde{q}\to q}\sum_{n\geqslant 0}(e^{-2i\tilde{q}\{n-[(r-1)/2]\}}-e^{-2i\tilde{q}\{n+[(r+1)/2]\}})\right)e^{4Dt\cos q}\,dq\\&=\pi\sum_{0\leqslant n<r}I_{2n-r+1}(4Dt).\end{aligned} \tag{A5}$$

Similarly, we find that

$$\begin{aligned}\tilde{I}_2(r,t)&=\frac{\pi}{2}\sum_{0\leqslant n<r}\{I_{2n-r}(4Dt)+I_{2n-r+2}(4Dt)\}\\&=\pi\sum_{0\leqslant n<r}I_{2n-r}(4Dt),\end{aligned} \tag{A6}$$

$$\begin{aligned}\tilde{I}_3(r,t)&=\frac{\pi}{2}\sum_{0\leqslant n<r}[I_{2n-r-1}(4Dt)+I_{2n+r-1}(4Dt)\\&\quad+I_{2n-r+3}(4Dt)+I_{2n+r+3}(4Dt)]\\&=\pi\sum_{0\leqslant n<r}I_{2n-r-1}(4Dt).\end{aligned} \tag{A7}$$

With the help of the asymptotic behavior of Bessel functions and using the properties of the incomplete Γ functions [18], the asymptotic behavior ($Dt\gg 1$ and $Jt\gg 1$) of the following integrals is readily found:

$$\int_t^{\infty}dt'\frac{e^{-4Jt'}}{\sqrt{8\pi Dt'}}\sim\frac{e^{-4Jt}}{4J\sqrt{8\pi Dt}}\left(1-\frac{1}{8Jt}+O((Jt)^{-2})\right), \tag{A8}$$

$$\int_t^{\infty}dt'\frac{e^{-4Jt'}}{\sqrt{8\pi Dt'}8Dt'}\sim\frac{e^{-4Jt}}{4J\sqrt{8\pi Dt}}\left(\frac{1}{8Dt}-\frac{3}{64Jt}+O((Jt)^{-3})\right), \tag{A9}$$

$$\int_t^{\infty}dt'\frac{e^{-4Jt'}}{\sqrt{8\pi Dt'}(Dt')^2}\sim\frac{e^{-4Jt}}{4J\sqrt{8\pi Dt}}\left(\frac{1}{(Dt)^2}+O((Jt)^{-3})\right). \tag{A10}$$

A further result ($Dt\gg 1$ and $Jt\gg 1$) used in the evaluation of the asymptotic behavior of the density and the two-point correlation function (25, 59, 83–85)

$$\int_t^\infty e^{-4(J+D)t'} I_n(4Dt') \sim \frac{e^{-4Jt}}{4J\sqrt{8\pi Dt}} \Bigg\{ \left(1 - \frac{1}{8Jt} + O((Jt)^{-2})\right) - \left(n^2 - \frac{1}{4}\right)\left(\frac{1}{8Dt} - \frac{3}{64JDt^2} + O((Jt)^{-3})\right) + \left(n^2 - \frac{1}{4}\right)\left(n^2 - \frac{9}{4}\right)\left(\frac{1}{128D^2t^2} + O((Jt)^{-3})\right) + \cdots \Bigg\}. \tag{A11}$$

Finally, the calculation of the constants A_0, B_0, C_0, when $J>0$ is performed with help of the formula [18]

$$\int_0^\infty dx\, e^{-\alpha x} I_\nu(\beta x) = \frac{\beta^\nu}{\sqrt{\alpha^2-\beta^2}(\alpha+\sqrt{\alpha^2-\beta^2})^\nu}$$

$$\forall \quad \mathrm{Re}(\nu) > -1, \quad \mathrm{Re}(\alpha) > \mathrm{Re}|\beta|. \tag{A12}$$

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