

Phase coexistence and spatial correlations in reconstituting k -mer models

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In reconstituting k -mer models, extended objects that occupy several sites on a one-dimensional lattice undergo directed or undirected diffusion, and reconstitute—when in contact—by transferring a single monomer unit from one k -mer to the other; the rates depend on the size of participating k -mers. This polydispersed system has two conserved quantities, the number of k -mers and the packing fraction. We provide a matrix product method to write the steady state of this model and to calculate the spatial correlation functions analytically. We show that for a constant reconstitution rate, the spatial correlation exhibits damped oscillations in some density regions separated, from other regions with exponential decay, by a *disorder surface*. In a specific limit, this constant-rate reconstitution model is equivalent to a single dimer model and exhibits a phase coexistence similar to the one observed earlier in totally asymmetric simple exclusion process on a ring with a defect.

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I. INTRODUCTION

Driven diffusive systems (DDS) evolve under local stochastic dynamics where by some conserved quantity such as mass, energy, or charge is being driven through the system [1,2]. Compared to their equilibrium counterparts, these systems exhibit rich steady-state behavior [3–5], including phase separation [6,7] and condensation transition [8] in one dimension, boundary layers [3,9], localized shocks [10] and have found a wide range of applications such as transport in super-ionic conductors [11], protein synthesis in prokaryotic cells [12,13], traffic flow [14], biophysical transport [15,16], etc. Recently, DDS with two or more species have been studied [17]; some of these systems with more than one conserved quantities [18,19] also exhibit phase transition even in one dimension. It is argued in Ref. [7] that phase separation transition in DDS is related to the condensation transition in a corresponding zero-range process (ZRP) [8].

Driven diffusive systems show interesting steady-state behavior when the constituting objects are extended [20] in the sense that they occupy more than one lattice site and move together as a single object called k -mer, obeying hardcore constraints. In one dimension, a driven system involving monodispersed k -mers was studied to understand the physical mechanism of protein synthesis in prokaryotic cells [12]. For such a system, the time evolution of the conditional probabilities of the site occupation, starting from a known initial configuration has been calculated [21], and phase diagram for such systems has also been reported [13]. Other works on such systems include studying hydrodynamic equations governing the local density evolution [22] and the effect of inhomogeneities and defects [23–25]. Microscopic processes like reconstitution, if present, can generate k -mers of arbitrary lengths and facilitates the possibility of phase separation.

In a recent article [26] it was shown that diffusing and reconstituting k -mers can be mapped to an interacting box-particle system with two species of particles. This mapping helps us in finding the exact phase boundaries of the phase separation

transition in k -mer dynamics. Depending on the rate of the reconstitution dynamics, one can obtain a macroscopic long polymer (which corresponds to condensation of particles). At the same time, since the motion of k -mers depends on their size, the system might go to a phase where a large k -mer moves so slow that it generates a large number of vacancies in front of it—this would lead to condensation of the holes (0s). Of course, in special situations, one may encounter simultaneous condensation of particles and holes. In this article, we aim at calculating spatial correlation in reconstituting k -mer models. Spatial correlation functions, up to now, has been calculated for models with monodispersity, i.e., when all k -mers are of equal size [13,27,28]. It has been found that steady state of these models can be written in matrix product form and correlation function in these models oscillate in both space and time [28]. Interestingly, in the continuum limit, the scaling behavior of the spatial correlation is found to be the same as that obtained for a driven tonks gas [20,29]. Various polydispersed models consisting of k -mers of different sizes and hence as many conservation laws have also been studied [30–33]. Their phase behavior in general show strongly broken ergodicity and the dynamical critical behavior.

The above-mentioned matrix formulation for fixed size k -mers cannot describe the polydispersed systems where the k -mers change their lengths dynamically. In a monodispersed system, where all the k -mers are of equal length, the k -mer density automatically fixes the packing fraction of the lattice. In reconstituting k -mer models, however, the density of k -mers and packing fraction are unrelated and independently conserved. Thus, configurations on a lattice, though containing only 1s and 0s, cannot be expressed as before by matrix strings containing just D s (for 1s) and E s (for 0s)—an additional matrix must be introduced to identify each k -mer and to keep track of the conservation of k -mer density. It turns out that the additional conservation law plays an important role in determining the stationary and dynamical properties of reconstituting k -mer models. In this article we provide a formalism to write the stationary state of polydispersed k -mers in matrix product form and calculate the spatial correlation functions analytically. We show that when reconstitution occurs between k -mers of size k_1 and k_2 with rate $w_1(k_1)w_2(k_2)$, one can *always* write an infinite-dimensional representation of

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matrices in terms of the rate functions. However, some specific cases can be represented by finite-dimensional matrices. One such example is the constant-rate reconstitution (CRR) model, where reconstitution occurs with constant rate and monomers diffuse with a rate different from the other k -mers. We calculate spatial correlation functions of CRR model explicitly and find that they show damped oscillations in some parameter regime and decay exponentially in other regimes. The disorder line that separates these regimes is also calculated.

The article is organized as follows. In Sec. II we introduce the reconstituting k -mer models and develop the matrix formulation to calculate the steady-state weights of configurations from representing string of matrices. In Sec. III, we introduce the CRR model, which has a finite-dimensional matrix representation, and calculate the spatial correlation functions and the disorder line explicitly for a given diffusion rate. Also, in this section we show that the CRR model in a special limit exhibits phase coexistence similar to the one observed in asymmetric exclusion process with a single defect. Finally, we conclude and summarize the results in Sec. IV.

II. THE RECONSTITUTING k -MER MODEL

Let us consider a driven diffusive system of polydispersed k -mers on a one-dimensional periodic lattice involving the directed diffusion and reconstitution dynamics. Along with drift, the k -mers change their size through exchange of monomer units. It is assumed that the reconstitution dynamics does not allow complete fusion of monomers and, thus, not only the mass (the total length of the k -mers) but also the number of k -mers is conserved.

For completeness, we start with the model studied recently in Ref. [26]. Let us consider M number of k -mers on a one-dimensional periodic lattice of L sites labeled by the index $i = 1, 2, \dots, L$. The k -mers, each having different integer length, are also labeled sequentially as $m = 1, 2, \dots, M$.

A k -mer is a hard extended object that occupies k consecutive sites on a lattice, and can be denoted by a string of k consecutive 1s (here represented by 1^k). Thus, every configuration of the system can be represented by a binary sequence with each site i carrying a variable $s_i = 1$ or 0 denoting, respectively, whether the lattice site is occupied by a k -mer or not. The total number of vacancies (0s) in the system is N and, thus, the total length of the k -mers is $K = \sum_{m=1}^M k_m = L - N$ (total number of 1s). We define the free volume (or void density) as $\rho_0 = N/L$ and the k -mer number density as $\rho = \frac{M}{L}$. Thus, the packing fraction of the lattice (fraction of volume occupied by the k -mers) is $\eta = 1 - \rho_0 = K/L$.

We consider directed diffusion of k -mers; a k -mer of size k_m moves to its right neighbor (if vacant) with rate $u(k_m)$,

$$k_m 0 \xrightarrow{u(k_m)} 0 k_m \equiv 1^{k_m} 0 \xrightarrow{u(k_m)} 0 1^{k_m}. \quad (1)$$

Along with this, reconstitution occurs among neighboring k -mers where one of the k -mers may release a single unit (or monomer) which instantly joins the other k -mer (see Fig. 1). Note that, reconstitution dynamics acts only at the interface of *immobile* k -mers, which are expected to remain in contact

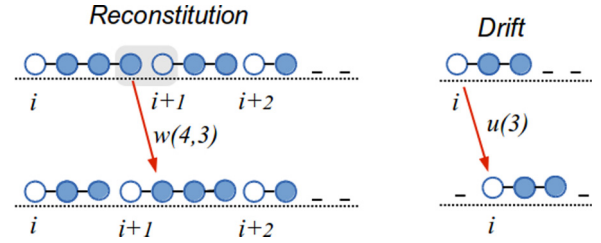


FIG. 1. Polydispersed k -mers in one dimension showing drift and reconstitution. Engine of the k -mers are marked as open circles. The drift rate $u(k)$ depends on the length of the corresponding k -mers. Reconstitution occurs only among consecutive immobile k -mers with a rate $w(k_i, k_{i+1})$, which depends on their lengths. An additional constraint $w(k, k') = 0$ for $k < 2$, conserves the number of k -mers in the system.

for long,

$$(k_m, k_{m+1}) \xrightleftharpoons[w(k_{m+1+1}, k_m-1)]{w(k_m, k_{m+1})} (k_m - 1, k_{m+1} + 1). \quad (2)$$

The reconstitution rate $w(k_m, k_{m+1})$ depends on the size of the participating k -mers and constrained by a condition $w(1, y) = 0$, which prohibits merging of k -mers and maintains the conservation of k -mer density ρ . It is evident that Eqs. (1) and (2) also conserve ρ_0 .

The dynamics of the model can be mapped exactly to a two-species generalization of misanthrope process (TMAP) [34] by considering each k -mer as a box containing $\kappa = k - 1$ particles of one kind (k -particles) and the number of consecutive vacancies (say n) in front of the k -mer as the number of particles of other type (0-particles). Thus, in TMAP, we have M boxes containing $\tilde{K} = K - M$ number of k -particles and N number of 0-particles.

From a box m containing (n_m, κ_m) number of 0- and k -particles, respectively, the particles hop to one of the neighboring boxes $m' = m \pm 1$ having $(n_{m'}, \kappa_{m'})$ particles with rates u_0 and u_k (respectively, for 0- and k -particles),

$$u_0(\kappa_m) = u(\kappa_m + 1)\delta_{m', m-1}, \\ u_k(\kappa_m, \kappa_{m'}) = w(\kappa_m + 1, \kappa_{m'} + 1)\delta_{n_m, 0}\delta_{n_{m'}, 0}. \quad (3)$$

The δ -function in the first equation forces 0-particles to move toward the left (same as k -mers moving to the right neighbor on the lattice) and those in the last equation take care of the restrictions that reconstitution (or exchange of k -particles) occurs among boxes m and m' only when they are devoid of 0-particles (equivalently, when k -mers are immobile).

It is well known that misanthrope processes enjoy the luxury of factorized steady state [35] for hop rates satisfying certain specific conditions. It is straight forward to derive similar conditions on hop rates of TMAP so that its steady state has a factorized form,

$$P(\kappa_i, n_i) = \frac{1}{Q_{\tilde{K}, N}} \prod_{i=1}^M f(\kappa_i, n_i) \\ \times \delta\left(\sum_i \kappa_i - \tilde{K}\right) \delta\left(\sum_i n_i - N\right), \quad (4)$$

where the δ functions ensure conservation of \tilde{K}, N , the total number of particles of each species, and $Q_{\tilde{K}, N}$ is the canonical partition function. When the reconstitution rate in k -mer model has a product form $w(k, k') = w_1(k)w_2(k')$, the hop rate of k -particles in corresponding TMAP [see Eq. (3)] also takes a product form $u_k(\kappa, \kappa') = w_1(\kappa)w_2(\kappa')$. For this simple choice, the weight function is given by [26]

$$f(\kappa, n) = \frac{1}{[u_0(\kappa)]^n} \prod_{\kappa'=1}^{\kappa} \frac{w_2(\kappa' - 1)}{w_1(\kappa')}. \quad (5)$$

Once the functional forms of $u(\cdot), w_1(\cdot), w_2(\cdot)$ are specified, one can calculate the steady-state properties of the TMAP exactly from the partition function in grand canonical ensemble (GCE) using two fugacities x and z for the conservation of \tilde{K} and N , respectively,

$$Z(x, z) = \sum_{\tilde{K}=0}^{\infty} \sum_{N=0}^{\infty} Q_{\tilde{K}, N} x^{\tilde{K}} z^N. \quad (6)$$

From this partition function, one can further calculate *one-point functions* of the k -mer models analytically. However, spatial correlation functions cannot be calculated straightforwardly. This is because the site variables $s_i = 1, 0$ on the k -mer model, which represent whether the site is occupied by a k -mer or not, are not so simple functions of the occupation numbers $\{n_i, \kappa_i\}$ of TMAP. We have

$$s_i = 1 - \sum_{j=1}^M \theta(g_j - i) \theta(i + 2 + n_j - g_j);$$

$$g_j = \sum_{l=1}^j (1 + n_l + \kappa_l), \quad (7)$$

where $\theta(x)$ is the Heaviside theta function. Clearly obtaining spatial correlation functions $C(r) = \langle s_i s_{i+r} \rangle - \langle s_i \rangle^2$ would be difficult (though not impossible) from the TMAP correspondence. In the following, we provide a matrix formulation to obtain the steady-state weight of any configuration of the k -mer model from a matrix string that uniquely represents that configuration.

A. Matrix product steady state

To calculate the spatial correlation functions explicitly and conveniently, in this section, we provide a matrix formulation similar to the one obtained earlier for exclusion processes having ZRP correspondence [36]. In Ref. [36], the authors showed that steady states of one-dimensional exclusion models having ZRP correspondence can be written in matrix product form—they also provided an infinite-dimensional representation of the matrices that can always be obtained from the corresponding ZRP weights [37]. In this article we try to obtain the spatial correlation functions of a polydispersed system in a similar way, i.e., by writing the steady-state weight of configuration as the trace of a representative matrix string.

How many matrices do we need? In ZRP, or its equivalent exclusion process, there was only one conserved quantity, which is the density or the packing fraction η . Here, we have an additional and independent conserved quantity ρ , the k -mer density. Thus, along with matrices D and E , which represent

the occupation status of a site we need another matrix, say A , that would appear once for every k -mer so that the k -mer number density is fixed appropriately. It is convenient to assign this matrix A to the left most site (or an engine) of a k -mer. In other words, every k -mer (1^k on a lattice) is represented by AD^{k-1} . In summary, in the matrix formulation, all occupied sites except the engine (A), are represented by matrix D s, and the vacant sites are represented by E s. Now, the steady-state weight of a configuration $\{n_i, \kappa_i\}$ can be expressed [using $\kappa_i = k_i - 1$ in Eq. (4)] as

$$\prod_{i=1}^M f(k_i - 1, n_i) = \text{Tr} \left[\prod_{i=1}^M AD^{k_i-1} E^{n_i} \right]. \quad (8)$$

We further assume that A can be expressed as an outer product of two vectors $A = |\alpha\rangle\langle\beta|$; the vectors $|\alpha\rangle, \langle\beta|$ and matrices D and E need to be determined from the dynamics. With this choice, Eq. (8) results in

$$f(k, n) = \langle\beta| D^k E^n |\alpha\rangle. \quad (9)$$

This equation is generic as long as the steady state of the TMAP corresponding to a reconstituting k -mer model has a factorized steady state. Now, any representation of $A = |\alpha\rangle\langle\beta|, D, E$ that satisfy Eq. (9) can provide a matrix product steady state for the k -mer model. One must, however, remember that any arbitrary matrix string does not necessarily represent a configuration of the k -mer model. Since every block of vacant sites (string of E s) must end with a k -mer represented by AD^{k-1} , all valid matrix strings must be devoid of ED . This brings in an additional constraint,

$$ED = 0, \quad (10)$$

which must be accounted for while searching a suitable matrix representation.

We now restrict ourselves to specific k -mer dynamics, which leads to a factorized steady state, as in Eq. (4). For the k -mer with hop rate $u(k)$ and reconstitution rate $\omega(k, k') = w_1(k)w_2(k')$, the steady state is given by Eq. (5). A set of matrices $\{\tilde{A}, \tilde{D}, \tilde{E}\}$ that satisfy Eq. (9),

$$\langle\tilde{\beta}| \tilde{D}^k \tilde{E}^n |\tilde{\alpha}\rangle = \frac{1}{[u(k+1)]^n} \prod_{k'=1}^k \frac{w_2(k' - 1)}{w_1(k')}, \quad (11)$$

is

$$|\tilde{\alpha}\rangle = \sum_{i=1}^{\infty} |i\rangle; \quad \langle\tilde{\beta}| = \langle 1|; \quad \tilde{D} = \sum_{i=1}^{\infty} \frac{w_2(i-1)}{w_1(i)} |i\rangle\langle i+1|$$

$$\tilde{E} = |1\rangle\langle 1| + \sum_{i=2}^{\infty} \frac{1}{u(i-1)} |i\rangle\langle i|, \quad (12)$$

where $\{|i\rangle\}$ with $i = 1, 2, \dots$ are standard basis vectors in infinite dimension. These matrices, however, do not satisfy Eq. (10). One option is to discard this representation and look for a new one that satisfy both Eqs. (10) and (9), which can be done in certain specific cases (see next section). But Eq. (12) is a general representation for k -mer models where k -mers drift with rate $u(k)$ and reconstitute with a rate having product form $w(k, k') = w_1(k)w_2(k')$. Thus, it would be beneficial to hold on to these matrices $\{\tilde{A}, \tilde{D}, \tilde{E}\}$ and to construct a new

representation using them, which satisfy both Eqs. (9) and (10). In this context, the following representation works:

$$|\alpha\rangle = |\tilde{\alpha}\rangle \otimes (|\tilde{1}\rangle + |\tilde{2}\rangle), \quad \langle\beta| = \langle\tilde{\beta}| \otimes \langle\tilde{2}|, \\ D = \tilde{D} \otimes |\tilde{2}\rangle\langle\tilde{2}|, \quad E = \tilde{E} \otimes (|\tilde{1}\rangle + |\tilde{2}\rangle)\langle\tilde{1}|. \quad (13)$$

Here, $\{|\tilde{1}\rangle, |\tilde{2}\rangle\}$ are the standard (and complete) basis vectors in two dimensions. More explicitly, we have

$$A = \begin{pmatrix} 0 & \tilde{A} \\ 0 & \tilde{A} \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ 0 & \tilde{D} \end{pmatrix}, \quad E = \begin{pmatrix} \tilde{E} & 0 \\ \tilde{E} & 0 \end{pmatrix}. \quad (14)$$

This infinite-dimensional representation provides a matrix product steady state for drifting and reconstituting k -mers in one dimension as long as the reconstitution rate has a product form. In the following, we illustrate a specific case where the representation is finite-dimensional.

III. CONSTANT-RATE RECONSTITUTION (CRR) MODEL

In this section we study a specific example of reconstituting k -mer model and illustrate the matrix product formulation presented in the previous section. Let us consider that the k -mers drift to their right neighbor with rate $u(k) = 1 + (v - 1)\delta_{k,1}$, i.e., the monomers ($k = 1$) move with rate v , whereas other k -mers move with unit rate. Let the reconstitution rate be a constant ω , independent of the size of the k -mers. In this constant-rate reconstitution (CRR) model matrices $\{\tilde{A}, \tilde{D}, \tilde{E}\}$, which satisfy only Eq. (9), have two-dimensional representations,

$$\tilde{A} = \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad \tilde{D} = \omega \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \quad \tilde{E} = \begin{pmatrix} \frac{1}{v} & 0 \\ 0 & 1 \end{pmatrix}. \quad (15)$$

However, since these matrices do not satisfy Eq. (10), we now construct new matrices $\{A, D, E\}$, using Eqs. (13) or (14),

$$A = \sum_{i=1}^4 |i\rangle\langle 3|, \quad D = \omega \sum_{i=3}^4 |i\rangle\langle 4|, \\ E = \sum_{i=1}^2 \left(\frac{1}{v} |2i-1\rangle\langle 2i-1| + |2i\rangle\langle 2i| \right), \quad (16)$$

which are four-dimensional, and represent, respectively, the engine of the k -mer, any other unit of the k -mer, and the vacancies 0s.

To calculate the correlation function and the densities, as usual, we start with the partition function in GCE, $Z = \text{Tr}[T^L]$, where the transfer matrix $T = A + xD + zE$. The fugacities z and x together control the densities ρ_0 and $\rho_d = 1 - \rho - \rho_0$, representing density of E s and D s, respectively. In fact, in this problem, the transfer matrix $T \equiv T(z, x, \omega, v)$ does not depend independently on x and ω , rather it depends on their product. Thus, any particular value of ω only redefines the fugacity $x \rightarrow x\omega$ and we can set $\omega = 1$ without loss of generality. Now, the partition function in GCE:

$$Z(z, x) = \text{Tr}(T^L); \\ T = A + xD + zE = \begin{pmatrix} z\tilde{E} & \tilde{A} \\ z\tilde{E} & x\tilde{D} + \tilde{A} \end{pmatrix}. \quad (17)$$

The characteristic equation for the eigenvalue of T is $\lambda f(\lambda) = 0$, with

$$f(\lambda) = xz(1 - v - z) + \{v + z + x(1 + v)\}z\lambda \\ - \{z + v(1 + x + z)\}\lambda^2 + v\lambda^3. \quad (18)$$

Thus, one of the eigenvalues of T is 0 and the other three, denoted by the largest eigenvalue λ_{\max} , and $\lambda_{1,2}$, are roots of the cubic polynomial $f(\lambda)$. The partition function in GCE is then

$$Z(z, x) = \lambda_{\max}(z, x)^L + \lambda_1(z, x)^L + \lambda_2(z, x)^L \\ \simeq \lambda_{\max}(z, x)^L, \quad (19)$$

where in the last step we have taken the thermodynamic limit $L \rightarrow \infty$. The conserved densities of the canonical ensemble are now

$$\rho_d = x \frac{\partial}{\partial x} \ln \lambda_{\max}, \quad \rho_0 = z \frac{\partial}{\partial z} \ln \lambda_{\max}. \quad (20)$$

This density fugacity relation specify the values of (z, x) , which uniquely correspond to a particular pair of conserved densities (ρ_0, ρ_d) . Any other observable in GCE, which are functions of (z, x) , can be expressed in terms of the densities (ρ_0, ρ_d) using Eq. (20). We must mention that densities can also be obtained as follows:

$$\rho_d = \langle d_i \rangle = x \frac{\text{Tr}[DT^{L-1}]}{\text{Tr}[T^L]}; \\ \rho_0 = \langle e_i \rangle = z \frac{\text{Tr}[ET^{L-1}]}{\text{Tr}[T^L]}; \quad (21) \\ \rho = \langle a_i \rangle = \frac{\text{Tr}[AT^{L-1}]}{\text{Tr}[T^L]}.$$

Here e_i, a_i, d_i are site variables that are unity when the site i is vacant, occupied by an engine, or by other units of a k -mer, respectively; otherwise, e_i, a_i, d_i are 0. In the thermodynamic limit, these definitions of densities are equivalent to Eq. (20).

A. Correlation functions

Now, we proceed to calculate the two-point correlation functions. The engine-engine correlation function is

$$C(r) = \langle a_i a_{i+r} \rangle - \langle a_i \rangle^2 = \frac{\text{Tr}[AT^{r-1}AT^{L-r-1}]}{\text{Tr}[T^L]} - \rho^2, \quad (22)$$

which, in the thermodynamic limit, can generically be expressed as

$$C(r) = p_1(z, x; v) \left(\frac{\lambda_1}{\lambda_{\max}} \right)^r + p_2(z, x; v) \left(\frac{\lambda_2}{\lambda_{\max}} \right)^r, \quad (23)$$

where p_1 and p_2 are independent of r . The behavior of the correlation functions depend on the nature of eigenvalues $\lambda_{1,2}$, which can be determined from the properties of the characteristic function $f(\lambda)$, in Eq. (18). When the eigenvalues $\lambda_{1,2}$ are real, ordered as $\lambda_{\max} > |\lambda_1| > |\lambda_2|$, the system has two length scales $|\ln \frac{|\lambda_{1,2}}{\lambda_{\max}}|^{-1}$ and the asymptotic form of the

correlation function is dominated by the largest one, $\xi = |\ln \frac{|\lambda_1|}{\lambda_{\max}}|^{-1}$. Correspondingly, the correlation has a monotonic exponential decay,

$$C(r) \simeq p_1(z, x; v) e^{-r/\xi}. \quad (24)$$

Also, in some parameter zone eigenvalues $\lambda_{1,2}$ may become complex. As they appear as complex conjugates we write $\lambda_{1,2} = \bar{\lambda} e^{\pm i\theta}$, with $\bar{\lambda} < \lambda_{\max}$. In this regime, $p_{1,2}$ defined in Eq. (23) must be complex conjugates $p_{1,2} = \bar{p} e^{\pm i\phi}$ so that the correlation function $C(r)$ is real. Consequently, $C(r)$ shows a damped oscillation, with a generic functional form

$$C(r) = \bar{p} e^{-r/\xi} \cos(\theta r + \phi), \quad (25)$$

where $\xi^{-1} = |\ln \frac{\bar{\lambda}}{\lambda_{\max}}|$.

It is interesting to note that a damped oscillation of the radial distribution function is a typical feature of a system in liquid phase, in contrast to the exponential decay of the same in the vapor phase. Naively one would think that such a change is a direct consequence of an underlying liquid-vapor phase transition. However, this is not the scenario in CRR model; possibility of a phase transition is ruled out here as the largest eigenvalue λ_{\max} is nondegenerate for any x, v, z and the corresponding free energy $\ln \lambda_{\max}$ would not be nonanalytic anywhere. This phenomena, a macroscopic change in the nature of correlation function in the absence of any phase transition, has been known for a while in literature, in different contexts, under the name of *disorder points* (or *lines*). In a broad sense, the *disorder points* separate the regions in parameter space showing qualitatively different pair correlation functions and were first introduced by Stephenson [39]. For Ising chains with ferromagnetic nearest-neighbor and antiferromagnetic next-nearest-neighbor interaction, the spin-spin correlation function in the disordered paramagnetic phase ($T > T_c$) shows damped oscillations when T is larger than T_D (the disorder point), whereas it decays exponentially for $T_c < T < T_D$ [40]. There are several other lattice spin models [41,42] that exhibit disorder lines. In context of fluids, a similar behavior has been observed in the decay of density profiles and the radial distribution functions—here the disorder lines that separate different regimes are conventionally termed as Fisher-Widom lines [43,44]. Recent studies also indicate existence of disorder lines in phenomenological models of QCD at finite temperature and density [45].

In CRR model, there are three parameters—the monomer diffusion rate v and the fugacities x, z (or alternatively the densities ρ, η). Thus, we have a two-dimensional *disorder surface* that separates the regimes of exponential decay from that of the damped oscillatory correlation functions in the (x, v, z) space. To identify the disorder surface we study the generic features of the characteristic function $\lambda f(\lambda)$ taking help of the Descartes's sign rule. Since all the parameters x, v, z are positive, Descartes's sign rule indicates that there is exactly one negative root when $z + v < 1$ irrespective of the value of x . In this regime, the root other than λ_{\max} must be real, as complex roots are generated pairwise. In the region $z + v > 1$, we have at most three positive roots: one positive and two complex or all positive; the disorder surface that separates these regimes in (x, v, z) space is shown in Fig. 2. In the

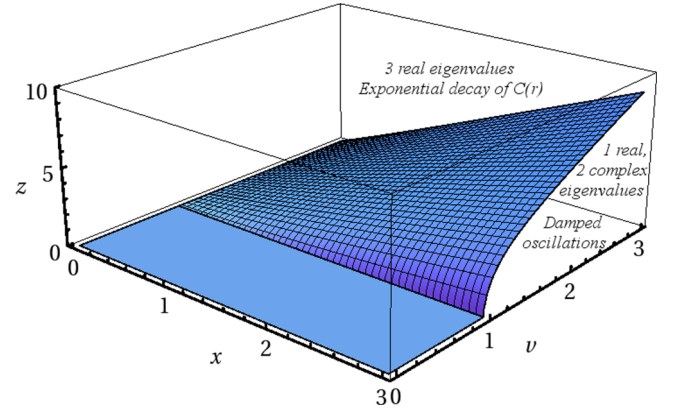


FIG. 2. Disorder surface separating regions where pair correlation function $C(r)$ decays exponentially (all three eigenvalues are real) from regions having damped oscillations (where the subdominant eigenvalues are complex).

region where the subdominant eigenvalues are “complex,” i.e., $\lambda_{1,2} = \bar{\lambda} e^{\pm i\theta}$ with $\bar{\lambda} < \lambda_{\max}$, the correlation function exhibits damped oscillations.

The exact analytic expression of eigenvalues, densities, and the two-point correlation functions are rather lengthy. For the purpose of illustration, we provide the details in the next section, for the CRR model only with $v = 2$, which lead to both decaying and oscillating correlation functions in different density regimes separated by a disorder line.

B. CRR model with $v = 2$

In this subsection we focus on the CRR model for a special case $v = 2$. We have already set the reconstitution rate $\omega = 1$, thus the grand canonical partition function depends only on two parameters z and x , which fix the densities ρ_0 and ρ_d . The packing fraction, which is defined as the fraction of the lattice occupied by k -mers, is now $\eta = \rho + \rho_d = 1 - \rho_0$. For $v = 2$, the eigenvalues are given by

$$\{\lambda_{\max}, \lambda_1, \lambda_2\} = \{g(1), g(\Omega), g(\Omega^2)\}, \quad (26)$$

where $g(y) = a + sy - \frac{p}{s}y^2$ and $\Omega = e^{i\pi/3}$. The other parameters are $a = 3z + 2x + 2$, $p = 4(1+x)^2 + 3z(z-2x)$, $q = 8(1+x)^3 + 9z(z-2x)(x-2z)$, and $s^3 = q + \frac{1}{2}\sqrt{4q^2 - p^3}$. The k -mer number density $\rho = 1 - \rho_0 - \rho_d$ and the packing fraction $\eta = 1 - \rho_0$ are now calculated from Eq. (20),

$$\rho = \frac{(2\lambda_{\max} - z)(\lambda_{\max} - z)(\lambda_{\max} - x)}{\lambda_{\max}(6\lambda_{\max}^2 - 2\lambda_{\max}(3z + 2x + 2) + z^2 + 2z + 3xz)}$$

$$\eta = \frac{\lambda_{\max}(2\lambda_{\max} - z)(\lambda_{\max} - z) + xz}{\lambda_{\max}(6\lambda_{\max}^2 - 2\lambda_{\max}(3z + 2x + 2) + z^2 + 2z + 3xz)}. \quad (27)$$

In Fig. 3 we have plotted η and ρ as a function of z , for different $x = 0.01, 0.1, 1$, and 10 , respectively, in Figs. 3(a) and 3(b).

As expected, for $z = 0$, the packing fraction is $\eta = 1$, independent of the fugacity x . On the other hand, in the limit $x \rightarrow 0$, it appears that both η and ρ might become discontinuous at $z = 2$ leading to a possibility of phase

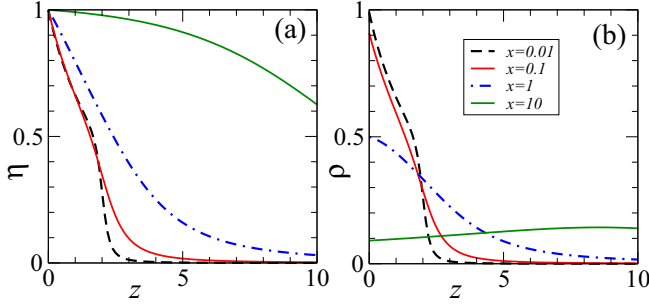


FIG. 3. Densities: (a) packing fraction η and (b) k -mer density ρ , as a function of z for $x = 0.01, 0.1, 1, 10$.

coexistence. In fact, *this* seems to be the case for any $v > 1$, and we discuss this possibility separately in the next section in details.

We now proceed to calculate the two-point correlation functions, first the engine-engine correlation function $C(r)$ defined in Eq. (22). If we formally write the densities in Eq. (27) as functions of z, x and λ_{\max} , as $\rho \equiv \hat{\rho}(z, x; \lambda_{\max})$ and $\eta \equiv \hat{\eta}(z, x; \lambda_{\max})$, the engine-engine correlation function, calculated using Eq. (22), can be written as

$$C(r) = \langle a_i a_{i+r} \rangle - \rho^2 = \rho \left[\hat{\rho}(z, x; \lambda_1) \left(\frac{\lambda_1}{\lambda_{\max}} \right)^r + \hat{\rho}(z, x; \lambda_2) \left(\frac{\lambda_2}{\lambda_{\max}} \right)^r \right]. \quad (28)$$

Also, the density-density correlation function $\langle s_i s_{i+r} \rangle - \eta^2$ takes a form similar to the right-hand side of the above equation with $\rho \rightarrow \eta$ and $\hat{\rho}(\cdot) \rightarrow \hat{\eta}(\cdot)$. Clearly, $C(r)$ will exhibit damped oscillations when $\lambda_{1,2} = \bar{\lambda} e^{\pm i\theta}$ are complex. Whether such a regime, separated from the usual exponential decay by a disorder line, exists for $v = 2$, can be determined from the characteristic polynomial $\lambda f(\lambda)$. The discriminant of the $f(\lambda)$ vanishes for $x = z/2$, which is the disorder line for $v = 2$ [as shown in Fig. 4(a)]; correspondingly, the disorder

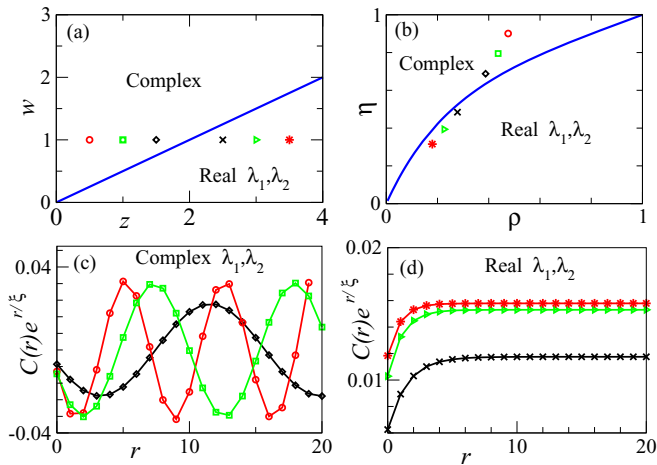


FIG. 4. Correlation functions: (a) For $v = 2$, complex roots appear for $x > z/2$, (b) the corresponding line in ρ - η plane, (c) engine-engine correlation function $C(r)$ for $z = \frac{1}{2}, 1, \frac{3}{2}$, and (d) $z = \frac{5}{2}, 3, \frac{7}{2}$. For (c) and (d), we use $x = 1$, and the symbols used here for different z are also marked in (a) and (b).

line in η - ρ plane [shown in Fig. 4(b)] is

$$\eta = \frac{\rho(\rho^2 + 3)}{(\rho + 1)^2}. \quad (29)$$

Thus, for $\eta > \frac{\rho(\rho^2 + 3)}{(\rho + 1)^2}$ the correlation functions are expected to have damped oscillatory behavior, whereas in the other regions the correlation functions must decay exponentially as a function of r .

To illustrate this, we take $x = 1$, which indicates that the correlation functions must be oscillatory for any $z < 2$. In Figs. 4(c) and 4(d) we have plotted $C(r)e^{r/\xi}$ as a function of r for $z = \frac{1}{2}, 1, \frac{3}{2}$ and $z = \frac{5}{2}, 3, \frac{7}{2}$, respectively. All these (z, x) values are shown as symbols in Fig. 4(a). The corresponding densities are shown in η - ρ plane, marked as same symbols [in Fig. 4(b)]. Clearly, $C(r)e^{r/\xi}$ shows oscillations when $z < 2$, whereas it asymptotically approaches to a constant when $z > 2$. It appears that existence of disorder lines is a generic feature in extended systems; this may be a consequence of the hardcore restriction among k -mers, which mimics a short-range repulsion existing in model fluids.

We close this section with the following interesting remarks.

Remark 1. The four-dimensional representation in CRR model leads to a transfer matrix T with $\text{Det}[T] = 0$. This in turn means that one of the eigenvalues $\lambda = 0$, indicating that there might be a three-dimensional representation that satisfies the matrix algebra Eqs. (9) and (10). We are able to find one such representation,

$$A = \begin{pmatrix} 1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \omega & \omega \end{pmatrix}, \quad (30)$$

$$E = \begin{pmatrix} \frac{1}{v} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

It is easy to check that $T = A + xD + zE$ gives the same characteristic polynomial $f(\lambda)$ as in Eq. (18).

Remark 2. For CRR model with $v = 2$, the line $x = z/2$, which separates regions having damped oscillations from regions with exponentially decaying correlations, is very special. On this line the engine-engine correlation function $C(r)$ vanishes, whereas the density-density correlation function remains finite. This can be verified from directly calculating the eigenvalues on this line, which are $\lambda_{\max} = 1 + 2x$ and $\lambda_1 = x = \lambda_2$. This makes the coefficients $\hat{\rho}(z, x; \lambda_{1,2}) = 0$ in Eq. (28).

Remark 3. This formulation is inadequate to calculate spatial correlation functions of k -mer models when reconstitution is absent. Naively one may think, setting $\omega = 0$ could work. But $\omega = 0$ would impose a condition $\langle \beta | D^k E^n | \alpha \rangle = 0$ for all k, n , which forces the weight of every configuration $\text{Tr}[\dots AD^k E^n A \dots]$ to vanish. In fact, when $\omega = 0$, diffusion of k -mers (of different size) is the only dynamics on the lattice, which keeps the initial ordering of their size invariant. Now the configuration space has infinitely many *disconnected ordering-conserving sectors*, and one must write partition sums separately for each sector.

Remark 4. In contrast to constant-rate reconstitution model, one may define a constant-rate diffusion model considering $u(k) = v$, a constant. Now, let us consider a reconstitution rate $\omega(k, k') = 1 + (\omega - 1)\delta_{k,2}\delta_{k',1}$, where dimers reconstitute with monomers at rate ω where as any other two k -mers reconstitute with unit rate. In this constant-rate diffusion model we have a simple two-dimensional representation:

$$A = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ w & 1 \end{pmatrix}, \quad E = \begin{pmatrix} \frac{1}{v} & 0 \\ 0 & 0 \end{pmatrix}. \quad (31)$$

In a two-dimensional representation both eigenvalues of $T = A + xD + zE$ (which is a positive matrix) are real and hence possibility of oscillatory feature in spatial correlation functions is ruled out.

C. Phase coexistence in CRR model in $x \rightarrow 0$ limit

In this section we investigate the CRR model in $x \rightarrow 0$ limit. We have seen in the previous section that for $v = 2$, the k -mer density ρ shows a sharp drop at $z = 2$. In fact, this feature is quite generic for all $v > 1$. When the fugacity x associated with D s approaches 0, we expect a microscopic number of D s in the system. In other words, most k -mers are only monomers. Thus, the best case scenario that represents $x \rightarrow 0$ limit is a system with *one* single D . Since this D must be associated with an engine A , we have exactly one dimer in the system that diffuses in the system with unit rate, and all other k mers are monomers diffusing with rate v . Thus, the dimer can be considered as a defect particle in the system. The reconstitution can occur only between this dimer and an adjacent monomer (when both are immobile) with rate $\omega = 1$. In this case, the reconstitution is equivalent to exchange of a monomer and a dimer.

Representing the single dimer as 2 and the monomers as 1s, and vacancies as 0s, the dynamics of the system can be written as

$$10 \xrightarrow{v} 01; \quad 20 \xrightarrow{1} 02; \quad 211 \xrightarrow{1} 121. \quad (32)$$

Since this dynamics is only a special case of the CRR model, we can proceed with the 4×4 representation given in Eq. (16). However, in this case there is a valid two-dimensional representation, because the weight of every configuration of the system can be written here as $\text{Tr}[AD \prod_{j=1}^{L-2} X_j]$, with X_j being either E or A . Clearly, these matrix strings do not contain ED and one need not bother about the constraint $ED = 0$ in Eq. (10) and can work with the 2×2 matrices $\{\tilde{A}, \tilde{D}, \tilde{E}\}$. In other words, the dimer, monomer, and vacancy are now represented by $D_2 = \tilde{A}\tilde{D}$, $D_1 = \tilde{A}$, and \tilde{E} , respectively. In GCE, the partition function is now

$$Z = \text{Tr}[D_2 T^{L-2}]; \quad T = z\tilde{E} + D_1 = \begin{pmatrix} 1 + z/v & 0 \\ 1 & z \end{pmatrix}. \quad (33)$$

The eigenvalues of T are $\{z, 1 + \frac{z}{v}\}$ and thus, for $v > 1$ the maximum eigenvalue changes from being $\lambda_{\max} = 1 + \frac{z}{v}$ to $\lambda_{\max} = z$ at a critical fugacity $z_c = \frac{v}{v-1}$. So, the partition

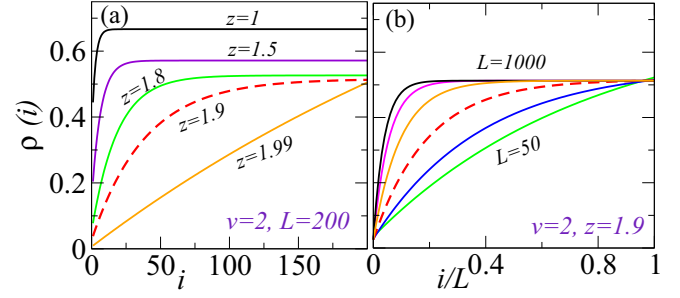


FIG. 5. (a) The density profile $\rho(i)$: (a) for $L = 200$, $v = 2$, and different $z = 1, 1.5, 1.8, 1.9, 1.99$. For small z , $\rho(i)$ saturates to the macroscopic bulk density $v/(v+z)$. For large z near z_c , such a saturation can be seen by increasing the system size L —this is shown in (b). The profile for $z = 1.9$ (marked as dashed line) as a function of i/L shows saturation as L increased.

function in the thermodynamic system $Z \sim \lambda_{\max}^L$ is non-analytic at $z = z_c$, indicating a phase transition.

First we calculate the density profile, as seen from the defect, which can be expressed as

$$\rho(r) = \frac{\text{Tr}[D_2 T^r D_1 T^{L-3-r}]}{\text{Tr}[D_2 T^{L-2}]} = \frac{\gamma}{z} \frac{z\gamma^r - z_c}{z\gamma^{L-2} - z_c}, \quad (34)$$

where r is distance from the defect site (or the dimer) and $\gamma = \frac{vz}{v+z}$ the ratio of eigenvalues. Thus, when $z < z_c$ or $\gamma < 1$, the profile $\rho(r)$ has a boundary layer in front of the defect site, which extends over a length scale $1/|\ln \gamma|$ and for large $r \ll L$, it saturates to a value $\rho_s = \gamma/z = v/(v+z)$. Thus, for a thermodynamically large system, the bulk of the system has a density $v/(v+z)$, which is the same as the expected monomer density in the thermodynamic limit,

$$\rho = 1 - z \frac{d}{dz} \ln \lambda_{\max} = \frac{v}{v+z}.$$

In Fig. 5(a) we have plotted $\rho(r)$ for different z considering $v = 2$ (corresponding bulk densities are $\rho_s = 2/(2+z)$). It is evident that for a small system (here $L = 200$) the boundary layer invades into the bulk as z approaches the critical value z_c . However, for any $z \lesssim z_c$, the boundary layer shrinks to $r = 0$ in the thermodynamic limit $L \rightarrow \infty$. This is shown in Fig. 5(b) for $z = 1.9$ (here $z_c = 2$) and $L = 50, 100, 200, 400, 700, 1000$.)

The fugacity z associated with the vacancies can tune the density of the monomers in the regime $z < z_c$, which corresponds to a density regime $\rho_c < \rho < 1$, where $\rho_c = 1 - 1/v$. In the canonical ensemble, if the conserved density is fixed at some value $\rho < \rho_c$, the system is expected to show phase coexistence. Since the allowed macroscopic densities are ρ_c and 0, and the average density has to be ρ , the system would allow a local density ρ_c in $\delta = \rho/\rho_c$ fraction of the lattice and keep $1 - \delta$ fraction vacant.

The single dimer problem we discussed here is very similar to the single defect in totally asymmetric simple exclusion process (TASEP) studied earlier in Refs. [46,47]. This TASEP model comprises a single defect particle (denoted by 2) and $L - 1$ normal particles (1s) on a ring of size L , following a

hopping dynamics,

$$10 \xrightarrow{1} 01; \quad 20 \xrightarrow{\alpha} 02; \quad 21 \xrightarrow{\beta} 12. \quad (35)$$

A special case of the model $\alpha = 1 = \beta$ [48] corresponds to a scenario where the defect 2 is a second-class particle, which helps in locating the shocks, if any. The model defined by the above dynamics can be solved using matrix product ansatz [5,46], but the matrices $\{E, D, A\}$ corresponding to $\{0, 1, 2\}$ have an infinite-dimensional representation, closely related to the matrices $\{E, D\}$ in TASEP [4]. A novel feature that arises in this model is the phase coexistence—for $\beta < \rho < 1 - \alpha$, the system shows a coexistence between a region of low-density β in front of the defect and a high-density $1 - \alpha$ behind it. Thus, a localized shock is formed at the site $j = \delta N$, such that the conserved density $\rho = \beta\delta + (1 - \alpha)(1 - \delta)$. In the following, we compare the phase coexistence scenario of this model with the single dimer model studied here.

The dynamics of the single dimer model, Eq. (32), is equivalent to

$$10 \xrightarrow{1} 01; \quad 20 \xrightarrow{1/v} 02; \quad 21 \xrightarrow[1/v]{1/v} 12. \quad (36)$$

However, in contrast to Eq. (35) there are two major differences in Eq. (36). First, the dimer occupies two lattice sites, whereas the defect particle 2 in exclusion processes occupies only one lattice site—this difference is not crucial in the thermodynamic limit. Second, in comparison to the defect dynamics in Eq. (35), (i) the dimer can exchange with a monomer in both directions, and (ii) the exchange occurs *only* when the immediate right neighbor of the exchanging sites is occupied.

If we overlook these differences, the models are similar when $\alpha = 1/v = \beta$. Thus, one may speculate that a phase coexistence may occur when $\frac{1}{v} < \rho < 1 - \frac{1}{v}$. In reality, however, for dynamics Eq. (32), phase coexistence occurs when $0 < \rho < \rho_c = 1 - \frac{1}{v}$. This similarity is striking—particularly when the matrix representation for Eq. (35) is infinite-dimensional, whereas the same for Eq. (32) is much simpler, 2×2 matrices.

IV. CONCLUSION

In this article we provide a general formulation to write the steady-state weights of reconstituting k -mer models in matrix product form. In the matrix formulation, we represent a vacancy by a matrix E , the engine of a k -mer (leading monomer unit from the left) by A and rest of the monomer units by D s. In these models, the k -mers, which are extended objects of different sizes, move to neighboring vacant sites with a rate that depends on their size. Reconstitution can occur among a pair of k -mers, when they are in contact, with a rate that depends on size of participating objects. Reconstitution usually means transfer of a monomer from one k -mer to the other one; we restrict such a transfer if length of the k -mer transferring a monomer is unity. This keeps the number of k -mers conserved. These models cannot be solved exactly for any arbitrary diffusion and reconstitution rates. Some of them can be solved, under quite general conditions, using a mapping of k -mer models to a two-species misanthrope process. These exactly solvable models, though simple, capture the different phases of the system and possible transitions among them

[26,49] quite well. However, calculating spatial correlation functions through this mapping is usually a formidable task, as the mapping does not keep track of the site-indices and the notion of distance. Thus, rewriting the steady-state weights in terms of a matrix product form is greatly useful.

If k -mers are monodispersed, i.e., each one has a fixed length k , the matrix product form is relatively simple [28]. This is because the density of k -mers ρ dictates the packing fraction $\eta = \rho k$, and one can get away with two matrices D and E representing whether the site is occupied or not. The fact that polydispersed systems studied here have *two* independent conserved quantities ρ and η brings in additional complications. First, to write the steady state in matrix product form, we need an additional matrix A (along with D, E) to identify the k -mers and to keep track of the conserved k -mer number. Next, additional care must be taken to ensure that every block of vacancies must end with A —in other words, all configurations must be devoid of ED .

In summary, the reconstituting k -mer models for which the steady-state weights can be obtained exactly through a two-species misanthrope process, we devise a matrix formulation to calculate spatial correlation functions explicitly. The required matrix algebra, and a generic representation that satisfies this algebra, are also provided. Specifically, we demonstrate the formulation for the constant-rate reconstitution (CRR) model, where reconstitution occurs with a constant rate ω , and all k -mers except the monomer move to its right neighbor (if vacant) with unit rate; the rate for monomers is $v \neq 1$. The two-point spatial correlation functions of CRR model show interesting behavior when k -mer density ρ and packing fraction η are tuned. In some density regime the spatial correlation functions show damped oscillation, whereas in other regimes they decay exponentially. The boundary that separates these regimes in ρ - η plane, conventionally known as the *disorder line*, is calculated analytically.

A special limit $\eta \rightarrow \rho$ of the CRR model is best represented by a system of monomers and a *single* dimer. The reconstitution process in this single dimer model is equivalent to exchange of a monomer with the dimer, when in contact. Effectively, the dimer behaves like a defect in the system and exhibits a phase coexistence, similar to the one observed in asymmetric exclusion processes with a single defect. We must mention that, though both models capture the phase separation scenario, the single dimer model is represented by a set of simpler 2×2 matrices in contrast to the infinite-dimensional representation in exclusion processes with a defect.

In this article we have considered directed diffusion of k -mers. This provides a natural interpretation that reconstitution occurs among immobile k -mers. However, the steady state and thus physical properties of the model are invariant if we use a symmetric diffusion of k -mers, and a reconstitution process that does not allow two particles of different species (in corresponding two species misanthrope process) to move out of a box simultaneously.

In this article we provide matrix product steady states for a class of k -mer models, by mapping them to a two-species misanthrope process. In fact, any two species misanthrope process can be mapped to a lattice containing extended objects—the steady state of such systems can *always* be

written in matrix product form. We believe that the matrix formulation developed here can be useful, in general, to

explore spatial correlation functions in extended systems in one dimension.

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