Phase coexistence and spatial correlations in reconstituting $k$-mer models

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In reconstituting $k$-mer models, extended objects which 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 polydisperse 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 behaviour \([3,4]\) including phase separation \([5,6]\) and condensation transition \([8]\) in one dimension, boundary layers \([5]\), 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 \([7]\) 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 \([22]\). Other works on such systems include studying hydrodynamic equations governing the local density evolution \([23]\) and the effect of inhomogeneities and defects \([24,25]\). Microscopic processes like reconstitution, if present, can generate $k$-mers of arbitrary lengths and facilitates the possibility of phase separation.

In a recent article \([27]\) we have 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 re-constitution 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 \([13,28,29]\). 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 \([29]\). Interestingly, in the continuum limit, the scaling behavior of the spatial correlation is found to be same as obtained for a driven tonks gas \([20,30]\). Various polydispersed models consisting of particles of different sizes and hence as many conservation laws have also been studied \([31,32]\). Their phase behavior in general show strongly broken ergodicity and the dynamical critical behavior.

The above mentioned matrix formulation for fixed size $k$-mers can not describe the polydispersed systems where the $k$ mers change their lengths dynamically. In a mono-dispersed 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 contain only 1s and 0s, can not be expressed as before by matrix strings containing just $Ds$ (for 1s) and $Es$ (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 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 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 section 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 section 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 section 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 [27]. Let us consider $M$ number of k-mers on a one dimensional periodic lattice of $L$ sites labeled by the index $i = 1, 2, ..., L$. The k-mers, each having different integer length, are also labeled sequentially as $m = 1, 2, ..., M$.

A k-mer is a hard extended object which 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 $\rho = M/L$. Thus the packing fraction of the lattice (fraction of volume occupied by the k-mers) is $\eta = 1 - \rho_0 = K/L$.

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 for long:

\[
(k_m, k_{m+1}) \xrightarrow{w(k_m, k_{m+1})/w(k_{m+1}, k_m-1)} (k_m - 1, k_{m+1} + 1). \tag{2}
\]

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 $\rho$. It is evident that Eqs. (1) and (2) also conserve $\rho_0$.

The dynamics of the model can be mapped exactly to a two-species generalization of misanthrope process (TMAP) [35] by considering each k-mer as the number of particles of other type (0-particles), $\mathcal{K}_L = K - M$ number of k-particles and $N$ number of 0-particles. From a box $m$ containing $(n_m, \kappa_m)$ number of 0- and k-particles respectively, the particles hop to one of the 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),

\[
u_0(\kappa_m) = u(\kappa_m+1)\delta_{m',m-1}
\nu_k(\kappa_m, \kappa_{m'}) = w(\kappa_m+1, \kappa_{m'}+1)\delta_{n_m,0}\delta_{n_{m'},0}. \tag{3}
\]

The $\delta$-function in the first equation forces 0-particles to move towards left (same as k-mers moving to the right

\begin{figure}[h]
\centering
\includegraphics[width=0.5\textwidth]{fig1.png}
\caption{(Color online) Poly-dispersed k-mers in one dimension showing drift and reconstitution. Engine of the k-mers are marked as orange. The rate of drift $u(k)$ 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.}
\end{figure}
neighboring on the lattice) and those in the last equation
take care of the restrictions that reconstitution (or ex-
change 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 [36] for hop rates satis-
ifying certain specific conditions. It is straightforward to
derive similar conditions on hop rates of TMAP so that
its steady state has a factorized form,

\[
P(\kappa_i, n_i) = \frac{1}{Q_{K,N}} \prod_{i=1}^{M} f(\kappa_i, n_i) \delta \left( \sum_i \kappa_i - K \right) \delta \left( \sum_i n_i - N \right),
\]

where the \( \delta \) functions ensure conservation of \( K \), \( N \), the
total number of particles of each species, and \( Q_{K,N} \) 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 corre-
ponding 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 [27],

\[
f(\kappa, n) = \frac{1}{[w_0(\kappa)]^n} \prod_{\kappa'}^{\kappa} \frac{w_2(k' - 1)}{w_1(k')}. \tag{5}
\]

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 \( K \) and \( N \) respectively,

\[
Z(x, z) = \sum_{K=0}^{\infty} \sum_{N=0}^{\infty} Q_{K,N} x^K z^N. \tag{6}
\]

From this partition function, one can further calculate
one-point functions of the \( k \)-mer models analytically.
However, spatial correlation functions cannot be calcu-
lated 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,

\[
s_i = 1 - \sum_{j=1}^{M} \theta(g_j - i) \theta(i + 2 + n_j - g_j); g_j = \sum_{l=1}^{j} (1 + n_l + \kappa_l);
\]

where \( \theta(x) \) is the Heaviside theta function. Clearly ob-
taining 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 which 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 for-
mulation similar to the one obtained earlier for exclusion
processes having ZRP correspondence [37]. In [37],
the authors showed that steady states of one dimensional
exclusion models having ZRP correspondence can be writ-
ten in matrix product form—they also provided an infinite
dimensional representation of the matrices that can al-
ways be obtained from the corresponding ZRP weights [38]. In this article we try to obtain the spatial cor-
relation functions of a polydisperse systems 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 equiv-
alent exclusion process, there was only one conserved
quantity, which is the density or the packing fraction \( \eta \).
Here, we have an additional and independent conserved
quantity \( \rho, \) the \( k \)-mer density. Thus along with mat-
crices \( D \) 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 ma-
trix \( A \) 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 \( Es \).
Now, the steady state weight of a configuration \( \{n_i, k_i\} \)
can be expressed (using \( \kappa_i = k_i - 1 \) in Eq. 4) as

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

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,

\[
f(k, n) = \langle \beta| D^{k} E^{n} |\alpha\rangle. \tag{9}
\]

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 ma-
trix 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 \( Es \))
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,

\[
ED = 0 \tag{10}
\]

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. (1). For the k-mer with hop rate \( u(k) \) and reconstitution rate \( \omega(k,k') = \omega_1(k)\omega_2(k') \), the steady state is given by Eq. (5). A set of matrices \( \{\tilde{A}, \tilde{D}, \tilde{E}\} \) that satisfy Eq. (9) are

\[
\langle \tilde{\beta} \rangle \tilde{D}^k \tilde{E}^n |\tilde{\alpha}\rangle = \frac{1}{[u(k+1)]^n} \prod_{k'=1}^{k} \frac{\omega_2(k'-1)}{\omega_1(k')} \quad (11)
\]

is

\[
|\tilde{\alpha}\rangle = \sum_{i=1}^{\infty} |i\rangle \langle 1|; \langle \tilde{\beta} | = \langle 1| \tilde{D} = \sum_{i=1}^{\infty} \frac{\omega_2(i-1)}{\omega_1(i)} |i\rangle \langle i+1| \quad (12)
\]

where \(|i\rangle\) with \( i = 1, 2 \ldots \) 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 (11), 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 \( w(k,k') = \omega_1(k)\omega_2(k') \). 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:

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

Here, \(|1\rangle, |2\rangle\) are the standard (and complete) basis vectors in 2-dimension. 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 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 \( \omega \), 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,

\[
\tilde{A} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \tilde{D} = \omega \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \quad \tilde{E} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 1 \end{pmatrix}. \quad (15)
\]

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

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

which are 4-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, \( Z = Tr[T^{k}] \) where the transfer matrix \( T = A + xD + zE \). The fugacities \( z \) and \( x \) together control the densities \( \rho_0 \) and \( \rho_d = 1 - \rho - \rho_0 \), representing density of Es and Ds respectively. In fact, in this problem, the transfer matrix \( T \equiv T(z, x\omega, v) \) does not depend independently on \( x \) and \( \omega \), rather depends on their product. Thus, any particular value of \( \omega \) only redefines the fugacity \( x \rightarrow x\omega \) and we can set \( \omega = 1 \) without loss of generality. Now, the partition function in GCE:

\[
Z(z, x) = Tr[T^{L}]; \quad T = A + xD + zE = \left( \begin{array}{cc} z\tilde{E} & \tilde{A} \\ \tilde{zE} & x\tilde{D} + \tilde{A} \end{array} \right). \quad (17)
\]

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

\[
Z(z, x) = \lambda_{\max}(z, x)^{L} + \lambda_{1}(z, x)^{L} + \lambda_{2}(z, x)^{L} \approx \lambda_{\max}(z, x)^{L} \quad (19)
\]

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 \( \rho_0, \rho_d \). Any other observable in GCE, which are functions of \( (z, x) \), can be expressed in terms of
the densities ($\rho_0, \rho_d$) using (20). We must mention that densities can also be obtained as follows.

$$\rho_d = \langle d_i \rangle = x \frac{Tr[DT^{L-1}]}{Tr[T^L]}, \quad \rho_0 = \langle e_i \rangle = z \frac{Tr[ET^{L-1}]}{Tr[T^L]},$$

$$\rho = \langle a_i \rangle = \frac{Tr[AT^{L-1}]}{Tr[T^L]}.$$

(21)

Here $e_i, a_i, d_i$ are site variables which 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

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

(22)

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

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

(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 $|\ln \frac{\lambda_1}{\lambda_{\max}}|^{-1}$ and the asymptotic form of the correlation function is dominated by the largest one, $C(r) \approx p_1(z, x; v) e^{-r/\xi}$. Correspondingly, the correlation has a monotonic exponential decay

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

(24)

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

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

(25)

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

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 $\lambda_{\max}$ is non-degenerate for any $x, v, z$ and the corresponding free energy $\ln \lambda_{\max}$ would not be non-analytic anywhere. This phenomena, a macroscopic change in the nature of correlation function in 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 [40]. For Ising chains with ferromagnetic nearest-neighbor and anti-ferromagnetic 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 $T_c < T < T_D$ [41]. There are several other lattice spin models [42, 43] 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 which separate different regimes are conventionally termed as Fisher-Widom lines [44, 45]. Recent studies also indicate existence of disorder lines in phenomenological models of QCD at finite temperature and density [46].

In CRR model, there are three parameters - the monomer diffusion rate $v$ and the fugacities $x, z$ (or alternatively the densities $\rho, \eta$). 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’ sign rule. Since, all the parameters $x, v, z$ are positive, Descartes’ sign rule indicate that there is exactly one negative root when $z + v < 1$ irrespective of the value of $x$. In this regime, the root other than $\lambda_{\max}$ must be real, as complex roots are generated pairwise. In the region $z + v > 1$, we have at most three positive roots: one posi-
tive 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 region where the sub-dominant eigenvalues are ‘complex’, i.e., \(\lambda_{1,2} = \lambda e^{\pm i\theta}\) with \(\lambda < \lambda_{\text{max}}\), 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 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 sub-section we focus on the CRR model for a special case \(v = 2\). We have already set the constitution rate \(\omega = 1\), thus the grand canonical partition function depends only on two parameters \(z\) and \(x\) which fix the densities \(\rho_0\) and \(\rho_d\). 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,

\[
\{\lambda_{\text{max}}, \lambda_1, \lambda_2\} = \{g(1), g(\Omega), g(\Omega^2)\}
\]

(26)

where \(g(y) = a + sy - 2y^2\) and \(\Omega = e^{i\pi/3}\). The other parameters are, \(a = 3z + 2x + 2\), \(p = 4(1+x)^2 + 3z(z-2x)\) and \(q = 8(1 + x)^3 + 9z(z - 2x)(x - 2z)\) and \(s^3 = q + \frac{1}{2}4y^2 - \rho^3\). 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),

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

\[
\eta = \frac{(2\lambda_{\text{max}} - z)(\lambda_{\text{max}} - z)(\lambda_{\text{max}} - x)}{\lambda_{\text{max}}(6\lambda_{\text{max}}^2 - 2\lambda_{\text{max}}(3z + 2x + 2) + z^2 + 2z + 3xz)}
\]

(27)

In Fig. 3 we have plotted \(\eta\) and \(\rho\) as a function of \(z\), for different \(x = 0.01, 0.1, 1\) and 10 respectively in (a) and (b). As expected, for \(z = 0\), the packing fraction is \(\eta = 1\), independent of the fugacity \(x\). On the other hand, in the limit \(x \to 0\), it appears that both \(\eta\) and \(\rho\) might become discontinuous at \(z = 2\) leading to a possibility of phase 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 \(z\) and \(\lambda_{\text{max}}\), as \(\rho \equiv \hat{\rho}(z, x; \lambda_{\text{max}})\) and \(\eta \equiv \hat{\eta}(z, x; \lambda_{\text{max}})\), the engine-engine correlation function, calculated using Eq. (22), can be written as

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

FIG. 3. (Color online) Densities: (a) Packing fraction \(\eta\) and (b) \(k\)-mer density \(\rho\), as a function of \(z\) for \(x = 0.01, 0.1, 1\) and 10.

\[
\eta = \frac{\rho(\rho^2 + 3)}{(\rho + 1)^2}
\]

(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 Fig. 4(c) and (d) we have plotted \(C(r)e^{r/\xi}\) as a function of \(r\) for \(z = \frac{1}{2}, 1, \frac{3}{2}\) and \(z = 2, 3, \frac{5}{2}\) respectively. All these \((z, x)\) values are shown as symbols in Fig. 4(a). The corresponding densities are are shown in \(\eta - \rho\) 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 \(\lambda = 0\),
inducing that there might be a three dimensional representation which satisfy the matrix algebra Eqs. [19] and [20]. We are able to find such a representation,

\[ A = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & \omega & \omega \end{pmatrix}, \quad E = \begin{pmatrix} \frac{1}{\nu} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

\[ \text{(30)} \]

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 \( \lambda_{\text{max}} = 1 + 2x \) and \( \lambda_1 = x = \lambda_2 \). This makes the co-efficients \( \tilde{\rho}(z, x; \lambda_{1,2}) = 0 \) 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 \( \omega = 0 \) would work. But \( \omega = 0 \) would impose a condition \( \langle \beta|D^kE^n|\alpha\rangle = 0 \) for all \( k, n \), which forces the weight of every configuration \( Tr[...A^kD^n...AE...] \) 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 \( \omega \) where as any other two \( k \)-mers reconstitute with unit rate. In this constant-rate diffusion model we have a simple two dimensional representation:

\[ A = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 \\ w & 1 \end{pmatrix}, \quad E = \begin{pmatrix} \frac{1}{\nu} & 0 \\ 0 & 0 \end{pmatrix}. \]

\[ \text{(31)} \]

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 \( x \to 0 \) limit

In this section we investigate the CRR model in \( x \to 0 \) limit. We have seen in the previous section that for \( v = 2 \), the \( k \)-mer density \( \rho \) 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 \( x \to 0 \) 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 which 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 \( 1 \)s, and vacancies as \( 0 \)s, the dynamics of the system can be written as

\[ 10 \xrightarrow{v} 01 ; \quad 20 \xrightarrow{1} 02 ; \quad 211 \xrightarrow{\nu} 121. \]

\[ \text{(32)} \]

Since this dynamics is only a special case of the CRR model, we can proceed with the \( 4 \times 4 \) representation given in Eq. (110). However, in this case there is a valid 2-dimensional representation, because the weight of every configuration of the system can be written here as \( Tr[AD \prod_{i=1}^{k=2} X_i] \), with \( X_i \) 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. (110) and can work with the \( 2 \times 2 \) matrices \( \{A, D, E\} \). In other words, the dimer, monomer and vacancy are now represented by \( D_2 \equiv A\tilde{D}, \; D_1 \equiv \tilde{A}, \) and \( E \) respectively. In GCE, the partition function is now

\[ Z = Tr[D_2 T_{\tilde{L}}^2]; \quad T = z\tilde{E} + D_1 = \begin{pmatrix} 1 + \frac{z}{\nu} & 0 \\ 0 & z \end{pmatrix}. \]

\[ \text{(33)} \]

The eigenvalues of \( T \) are \( \{z, 1 + \frac{z}{\nu}\} \) and thus, for \( v > 1 \) the maximum eigenvalue changes from being \( \lambda_{\text{max}} = 1 + \frac{z}{\nu} \) to \( \lambda_{\text{max}} = z \) at a critical fugacity \( z_c = \frac{\nu}{\nu - 1} \). So, the partition functions
Macroscopic densities are expected to show phase coexistence. Since the allowed fraction of the lattice and keep 1 − δ 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 [47, 48]. This TASEP model comprises of a single defect particle (denoted by 2) and L − 1 normal particles (1s) on a ring of size L, following a hopping dynamics,

\[ 10 \rightarrow 01 ; \quad 20 \rightarrow 02 ; \quad 21 \rightarrow 12. \]  

A special case of the model \( \alpha = 1 = \beta \) 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, 47], 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 \( \beta \) 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 \( \rho = \beta \beta + (1 - \alpha)(1 - \delta) \). 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

\[ 10 \rightarrow 01 ; \quad 20 \rightarrow 02 ; \quad 21 \rightarrow 12. \]  

However, in contrast to Eq. (35) there are two major differences in [49]. Firstly 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. Secondly, 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 (32), phase coexistence occurs when \( 0 < \rho < \rho_c = 1 - \frac{1}{v} \). This similarity is striking - particularly when the matrix representation for (35) is infinite dimensional whereas the same for (32) is much simpler, \( 2 \times 2 \) 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 \( Ds \). 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

---

function, in the thermodynamic system, \( Z \sim \lambda_{\text{max}}^L \) 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

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

where \( r \) is distance from the defect site (or the dimer) and \( \gamma = \frac{\ln \lambda_{\text{max}}}{v} \) is 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 same as the expected monomer density in the thermodynamic limit,

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

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 \( z \geq z_c \), 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 \( \rho_c \) and 0, and the average density has to be \( \rho \), the system would allow a local density \( \rho_c \) 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 [47, 48].
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 can not 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.\cite{27, 50} This is because, the density of useful.

state weights in terms of a matrix product form is greatly and the notion of distance. Thus, rewriting the steady tution rates. Some of them can be solved, under quite extended systems in one dimension.

If k-mers are mono-dispersed, i.e., each one has a fixed length k, the matrix product form is relatively simple\cite{29}. This is because, the density of k-mers ρ dictates the packing fraction \( \eta = p_k \), and one can get away with two matrices D and E representing whether the site is occupied or not. The fact, poly-dispersed systems studied here have two independent conserved quantities ρ and \( \eta \), 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 device 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 \( \omega \), and all k-

mers except the monomer, move to its right neighbour (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 \( \rho \) and packing fraction \( \eta \) 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 \( \rho-\eta \) plane, conventionally known as the disorder line, is calculated analytically.

A special limit \( \eta \to \rho \) 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 \( 2 \times 2 \) matrices in contrast to the infinite dimensional representation in exclusion processes with a defect.

In all through 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 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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