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On the structure factor of jammed particle configurations on the one-dimensional lattice

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Abstract. A broad class of blocked or jammed configurations of particles on the one-dimensional lattice can be characterized in terms of local rules involving only the lengths of clusters of particles (occupied sites) and of holes (empty sites). Examples of physical relevance include the metastable states reached by the zero-temperature dynamics of kinetically constrained spin chains, the attractors of totally irreversible processes such as random sequential adsorption, and arrays of Rydberg atoms in the blockade regime. The configurational entropy of ensembles of such blocked configurations has been investigated recently by means of an approach inspired from the theory of stochastic renewal processes. This approach provides a valuable alternative to the more traditional transfer-matrix formalism. We show that the renewal approach is also an efficient tool to investigate a range of observables in uniform ensembles of blocked configurations, besides their configurational entropy. The main emphasis is on their structure factor and correlation function.

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1. Introduction

Blocked or jammed configurations are met in many guises in the statistical physics of complex systems, including first and foremost glassy and granular materials (see [1, 2] for reviews). In this work we focus our attention onto blocked configurations of particles on the one-dimensional lattice. Various situations of physical significance involving such arrays of particles are recalled below.

Many examples of blocked configurations in one dimension correspond to the attractors of some underlying zero-temperature dynamics launched from an infinite-temperature disordered initial state. Within this setting, these blocked configurations may be viewed as one-dimensional zero-temperature analogues of the metastable states (also known as valleys, pure states, inherent structures, or quasi-states) which are met in higher-dimensional or mean-field models at finite temperature (see [3, 4] and references therein). A broad variety of kinetic spin models are known to have an exponentially large number of attractors consisting of single blocked or jammed configurations. This includes pristine models, such as the Ising chain with Kawasaki dynamics [5, 6], disordered models, such as the Ising spin glass [7, 8], and a breadth of kinetically constrained spin models [9, 10, 11, 12, 13, 14, 15, 16, 17]. Several lattice gas models share the same phenomenology [18, 19, 20, 21, 22]. The zero-temperature dynamics of the above models is irreversible and strongly non-ergodic. Some of these kinetic models can be exactly mapped onto the dynamics of the deposition of hard objects on the one-dimensional lattice. Prototypical examples are RSA (random sequential adsorption) or CSA (cooperative sequential adsorption), where particles or clusters are deposited irreversibly and sequentially on an initially empty substrate [23, 24, 25]. The process stops when no further object can be inserted into the system, which is left in a blocked or jammed configuration with a non-trivial density or coverage.

Another more recent motivation to investigate blocked configurations of particles defined by local constraints comes from an entirely different area, namely the physics of ultracold atoms. Trapped Rydberg atoms appear as a promising benchmark for what concerns quantum computation, simulation and information processing [26]. Their large size and strong interactions may give rise to a blockade, preventing the excitation of Rydberg atoms in the vicinity of an already existing one [27, 28, 29, 30, 31, 32]. In the simple setting of a one-dimensional optical lattice, each site occupied by a Rydberg atom must have at least b empty sites on either side, where $b \geq 1$ is referred to as the blockade range [33, 34]. To close this panorama with an example outside the realm of physics, we mention the Riviera model, where houses are sequentially built on an infinite array of pre-drawn plots along a beach, with the constraint that every house should enjoy the sunlight from at least one of the side directions. New houses are successively introduced until a blocked configuration is reached [35, 36, 37, 38].

A prominent quantity characterizing statistical ensembles of blocked configurations is their configurational entropy S_\star describing the exponential growth of the number $\mathcal{N}_N \sim \exp(NS_\star)$ of blocked configurations with the system size N . In many situations, the configurational entropy has been determined either by combinatorial means [12, 34, 39, 40, 41, 42, 43] or by the transfer-matrix approach [15, 17]. We have proposed a novel method to evaluate S_\star in a recent paper in collaboration with Krapivsky [44]. This approach, inspired from the theory of renewal processes, works whenever the rules defining blocked configurations involve only the lengths of clusters of particles and holes. Within this scope, which embraces most situations of physical

significance, the renewal approach is more systematic and easier to implement than the more traditional transfer-matrix approach.

The goal of the present work is to show that the same approach can be efficiently used to investigate a range of observables, besides the configurational entropy, of uniform ensembles of blocked configurations. The setup of this paper is as follows. Section 2 is devoted to generalities and to simple observables. We first recall the definition of the statistical ensembles introduced in [44] (section 2.1) and the determination of their configurational entropy by the renewal approach (section 2.2). In section 2.3 we use the same approach to investigate simple local observables, such as boundary probabilities and the length distributions of clusters of particles and holes. Section 3 is devoted to the main subject of this work, namely the structure factor and the correlation function of uniform ensembles. After recalling some definitions (section 3.1), we successively evaluate Fourier amplitudes (section 3.2), structure factors (section 3.3), and correlation functions (section 3.4), describing in some detail the general properties of these quantities. The next sections concern examples of ensembles of blocked configurations. Explicit results are derived in section 4 for the three simplest statistical ensembles already considered in [44]. We then consider the ensemble of attractors of the k -mer deposition model (section 5) and of arrays of Rydberg atoms with blockade range b (section 6). Single configurations pertaining to both models can be mapped onto each other, with the correspondence $k = b + 1$. A brief discussion is given in section 7. An appendix is devoted to the Hendricks-Teller model [45], a simple example of a random structural model whose structure factor can be studied by means of the renewal approach.

2. Model and simple observables

2.1. The model

Let us first recall the statistical model of blocked configurations introduced in [44]. Configurations are semi-infinite sequences of particles (or occupied sites, noted \bullet) and of holes (or empty sites, noted \circ). Such a configuration \mathcal{C} is described by the lengths $i_1, j_1, i_2, j_2, \dots$ of the successive clusters of particles and holes. It is therefore either of the form

$$\mathcal{C}_I = \underbrace{\bullet \dots \bullet}_{i_1} \underbrace{\circ \dots \circ}_{j_1} \underbrace{\bullet \dots \bullet}_{i_2} \underbrace{\circ \dots \circ}_{j_2} \dots \quad (2.1)$$

if the first site is occupied, or of the form

$$\mathcal{C}_J = \underbrace{\circ \dots \circ}_{j_1} \underbrace{\bullet \dots \bullet}_{i_1} \underbrace{\circ \dots \circ}_{j_2} \underbrace{\bullet \dots \bullet}_{i_2} \dots \quad (2.2)$$

if the first site is empty.

Blocked configurations are defined by the following local rules:

- All lengths i_1, i_2, \dots of particle clusters belong to some set \mathcal{I} of positive integers.
- All lengths j_1, j_2, \dots of hole clusters belong to some set \mathcal{J} of positive integers.

In the above, \mathcal{I} and \mathcal{J} are two prescribed finite or infinite subsets of the positive integers, which entirely define the configurational model. Hereafter we always deal with the uniform statistical ensemble obtained by attributing equal weights to all blocked configurations \mathcal{C} constructed as above. We assume that the model is non-trivial, namely that both sets \mathcal{I} and \mathcal{J} are non-empty and at least one of them contains more than one integer.

2.2. Configurational entropy

To set the stage, we begin by recalling the analysis of the configurational entropy. This quantity, denoted by S_* , describes the exponential growth

$$\mathcal{N}_N \sim \exp(NS_*) \quad (2.3)$$

of the number \mathcal{N}_N of configurations \mathcal{C}_N on a finite system of length N . No overhang is allowed in the construction, so that the rightmost cluster ends exactly at site N . We also introduce the numbers $\mathcal{N}_{N,I}$ and $\mathcal{N}_{N,J}$ of finite configurations $\mathcal{C}_{N,I}$ and $\mathcal{C}_{N,J}$ beginning with a cluster of particles or of holes, in correspondence with (2.1) and (2.2).

The key observation made in [44] is the existence of a formal analogy between the present setting and the theory of stochastic renewal processes [46, 47, 48] (see [49, 50] for presentations in the physics literature). According to their usual definition, renewal processes take place on the semi-infinite time axis ($t > 0$) and evolve from a given initial condition. Hence considering semi-infinite configurations with prescribed initial condition is the most appropriate framework for exploiting to the full the analogy between the present problem and renewal processes. From a more technical viewpoint, this analogy also leads one to introduce the generating series of the numbers of configurations

$$\begin{aligned} \mathcal{N}_I(z) &= \sum_{N \geq 1} \mathcal{N}_{N,I} z^N, & \mathcal{N}_J(z) &= \sum_{N \geq 1} \mathcal{N}_{N,J} z^N, \\ \mathcal{N}(z) &= \sum_{N \geq 0} \mathcal{N}_N z^N. \end{aligned} \quad (2.4)$$

We have

$$\mathcal{N}(z) = 1 + \mathcal{N}_I(z) + \mathcal{N}_J(z), \quad (2.5)$$

where the initial term $\mathcal{N}_0 = 1$ is conventional. The series $\mathcal{N}_I(z)$ and $\mathcal{N}_J(z)$ obey linear renewal equations of the form

$$\mathcal{N}_I(z) = I(z)(1 + \mathcal{N}_J(z)), \quad \mathcal{N}_J(z) = J(z)(1 + \mathcal{N}_I(z)), \quad (2.6)$$

where

$$I(z) = \sum_{i \in \mathcal{I}} z^i, \quad J(z) = \sum_{j \in \mathcal{J}} z^j \quad (2.7)$$

are the series associated with the sets \mathcal{I} and \mathcal{J} defining the statistical ensemble. Solving the linear equations (2.6), we obtain the results

$$\mathcal{N}_I(z) = \frac{I(z)(1 + J(z))}{1 - I(z)J(z)}, \quad \mathcal{N}_J(z) = \frac{J(z)(1 + I(z))}{1 - I(z)J(z)} \quad (2.8)$$

and

$$\mathcal{N}(z) = \frac{(1 + I(z))(1 + J(z))}{1 - I(z)J(z)}. \quad (2.9)$$

As z increases from 0 to 1, the product $I(z)J(z)$ increases from $I(0)J(0) = 0$ to $I(1)J(1) = |\mathcal{I}||\mathcal{J}| \geq 2$ (possibly infinite). There is therefore a single value z_* of z in the range $0 < z_* < 1$ such that the denominator of (2.9) vanishes, i.e.,

$$I(z_*)J(z_*) = 1. \quad (2.10)$$

The configurational entropy entering the exponential growth law (2.3) reads

$$S_* = -\ln z_*. \quad (2.11)$$

Throughout the following, along the lines of [44], we restrict this study to the rational class of models where both generating series

$$I(z) = \frac{A_I(z)}{B_I(z)}, \quad J(z) = \frac{A_J(z)}{B_J(z)} \quad (2.12)$$

are rational functions, i.e., ratios of polynomials in z . This class encompasses all examples considered below, and virtually all situations of physical significance (see [44] for more details). The formula (2.9) then takes the form

$$\mathcal{N}(z) = \frac{C(z)}{D(z)}, \quad (2.13)$$

where $C(z)$ and $D(z)$ are polynomials in z . The rational fraction (2.13) is assumed to be irreducible. The degree of $D(z)$ is denoted by Δ . Its smallest zero z_* is real, positive, and simple. The degree Δ provides a natural measure of the complexity of configurational models in the rational class.

2.3. Local observables

Our main goal is to show that the renewal method recalled above provides an efficient tool to evaluate a good deal of observables in the uniform ensemble, besides its configurational entropy. The case of the Hendricks-Teller model, considered in Appendix A, serves as a warming up for what follows. The remainder of this section is devoted to local observables such as boundary probabilities and the length distribution of particle and hole clusters. Section 3 will be about the main subject of this work, namely the structure factor and the correlation function.

Boundary probabilities. Our first observables are the boundary probabilities W_I (resp. W_J) that an infinitely long configuration \mathcal{C} begins with a cluster of particles (resp. a cluster of holes), i.e.,

$$W_I = \lim_{N \rightarrow \infty} \frac{\mathcal{N}_{N,I}}{\mathcal{N}_N}, \quad W_J = \lim_{N \rightarrow \infty} \frac{\mathcal{N}_{N,J}}{\mathcal{N}_N}. \quad (2.14)$$

We have $\mathcal{N}_N = \mathcal{N}_{N,I} + \mathcal{N}_{N,J}$ for $N \geq 1$, and so $W_I + W_J = 1$, as expected. All generating series entering (2.8) and (2.9) have poles at $z = z_*$, so that all numbers of configurations grow as $\exp(NS_*)$. We have therefore

$$W_I = \lim_{z \rightarrow z_*} \frac{\mathcal{N}_I(z)}{\mathcal{N}(z)}, \quad W_J = \lim_{z \rightarrow z_*} \frac{\mathcal{N}_J(z)}{\mathcal{N}(z)}. \quad (2.15)$$

The formulas (2.8) and (2.9) yield

$$\begin{aligned} W_I &= \frac{I(z_*)}{1 + I(z_*)} = \frac{1}{1 + J(z_*)}, \\ W_J &= \frac{J(z_*)}{1 + J(z_*)} = \frac{1}{1 + I(z_*)}. \end{aligned} \quad (2.16)$$

Distributions of cluster lengths and their moments. We now turn to the length distributions of the clusters of particles and of holes, i.e.,

$$p_{I,k} = \text{Prob}(i = k), \quad p_{J,k} = \text{Prob}(j = k), \quad (2.17)$$

where i (resp. j) stands for the length of any particle cluster (resp. any hole cluster) in an infinitely long configuration. Consider particle clusters for definiteness. All such clusters are interchangeable, so that we have

$$p_{I,k} = \text{Prob}(i_1 = k) = \lim_{N \rightarrow \infty} \frac{\mathcal{N}_{N,I,k}}{\mathcal{N}_{N,I}}, \quad (2.18)$$

where $\mathcal{N}_{N,I,k}$ is the number of configurations of length N beginning with a cluster of particles of length $i_1 = k$. The corresponding generating series reads

$$\mathcal{N}_{I,k}(z) = \sum_{N \geq 1} \mathcal{N}_{N,I,k} z^N = z^k \chi_I(k) (1 + \mathcal{N}_J(z)), \quad (2.19)$$

where

$$\chi_I(k) = \begin{cases} 1 & (k \in \mathcal{I}), \\ 0 & (k \notin \mathcal{I}) \end{cases} \quad (2.20)$$

is the indicator function of the set \mathcal{I} . In line with (2.15), we have

$$p_{I,k} = \lim_{z \rightarrow z_\star} \frac{\mathcal{N}_{I,k}(z)}{\mathcal{N}_I(z)}. \quad (2.21)$$

We thus obtain

$$p_{I,k} = \frac{z_\star^k}{I(z_\star)} \chi_I(k), \quad (2.22)$$

and similarly

$$p_{J,k} = \frac{z_\star^k}{J(z_\star)} \chi_J(k). \quad (2.23)$$

In particular, the mean lengths of particle and hole clusters read

$$\begin{aligned} \langle i \rangle &= \sum_{k \geq 1} k p_{I,k} = \sum_{k \in \mathcal{I}} \frac{k z_\star^k}{I(z_\star)} = \frac{z_\star I'(z_\star)}{I(z_\star)} = z_\star I'(z_\star) J(z_\star), \\ \langle j \rangle &= z_\star I(z_\star) J'(z_\star). \end{aligned} \quad (2.24)$$

Here and throughout the following, $\langle \cdot \rangle$ denotes an average over the uniform ensemble of blocked configurations. The mean distance between consecutive particle clusters (or, equivalently, between consecutive hole clusters) is therefore

$$\ell = \langle i \rangle + \langle j \rangle = z_\star (I'(z_\star) J(z_\star) + I(z_\star) J'(z_\star)). \quad (2.25)$$

The particle density can be obtained as

$$\rho = \frac{\langle i \rangle}{\ell} = \frac{I'(z_\star) J(z_\star)}{I'(z_\star) J(z_\star) + I(z_\star) J'(z_\star)}. \quad (2.26)$$

An equivalent expression was derived by another route in [44]. Higher moments of the cluster lengths can be determined along the same lines:

$$\begin{aligned} \langle i^p \rangle &= J(z_\star) \left(z \frac{d}{dz} \right)^p I(z) \Big|_{z=z_\star}, \\ \langle j^p \rangle &= I(z_\star) \left(z \frac{d}{dz} \right)^p J(z) \Big|_{z=z_\star}. \end{aligned} \quad (2.27)$$

We have especially

$$\begin{aligned} \langle i^2 \rangle &= z_\star J(z_\star) (I'(z_\star) + z_\star I''(z_\star)), \\ \langle j^2 \rangle &= z_\star I(z_\star) (J'(z_\star) + z_\star J''(z_\star)). \end{aligned} \quad (2.28)$$

3. General results on structure factor and correlation function

3.1. Definitions

Each configuration \mathcal{C} can be alternatively described by the occupation numbers

$$\eta_m = \begin{cases} 1 & \text{(site } m \text{ is occupied),} \\ 0 & \text{(site } m \text{ is empty).} \end{cases} \quad (3.1)$$

The correlation functions of the model are $\langle \eta_m \rangle$, $\langle \eta_m \eta_l \rangle$, and so on, where averages are taken over the uniform ensemble. Translation invariance and clustering of correlations hold in the bulk of the system, i.e., far from its boundary. We have in particular

$$\langle \eta_m \rangle \rightarrow \rho, \quad \langle \eta_m \eta_l \rangle - \langle \eta_m \rangle \langle \eta_l \rangle \rightarrow C_{m-l} \quad (3.2)$$

as m and l are simultaneously large, the difference $m-l$ being kept fixed. The particle density ρ is given by (2.26). The connected pair correlation function C_n is an even function of n which falls off to zero as the distance $|n|$ between both sites gets large. It is invariant under the exchange of particles and holes ($\eta_m \longleftrightarrow 1 - \eta_m$).

The (random) Fourier amplitude $G_N(q)$ and intensity $S_N(q)$ associated with the first N sites read

$$G_N(q) = \sum_{n=1}^N e^{-imq} \eta_m, \quad S_N(q) = \frac{|G_N(q)|^2}{N}. \quad (3.3)$$

Our main interest is in the structure factor

$$S(q) = \lim_{N \rightarrow \infty} \langle S_N(q) \rangle. \quad (3.4)$$

This self-averaging quantity identifies with the Fourier transform of the correlation function C_n :

$$S(q) = \sum_{n=-\infty}^{\infty} C_n e^{-inq}. \quad (3.5)$$

3.2. Fourier amplitudes

In order to determine the Fourier amplitudes, it is advantageous to split the definition (3.3), denoting by $G_{N,I}(q)$ (resp. $G_{N,J}(q)$) the Fourier amplitude of a finite configuration of type $\mathcal{C}_{N,I}$ (resp. $\mathcal{C}_{N,J}$). These amplitudes obey the renewal equations

$$\begin{aligned} G_{N,I}(q) &= a(i_1, q) + e^{-iqi_1} G_{N-i_1, J}(q), \\ G_{N,J}(q) &= e^{-iqj_1} G_{N-j_1, I}(q), \end{aligned} \quad (3.6)$$

with

$$a(i_1, q) = \sum_{m=1}^{i_1} e^{-imq} = \frac{e^{-iq}}{1 - e^{-iq}} (1 - e^{-iqi_1}). \quad (3.7)$$

In (3.6), the amplitude denoted by $G_{N-i_1, J}(q)$ is associated with the $N - i_1$ atoms of the configuration \mathcal{C}_I numbered from $i_1 + 1$ to N . It is a probabilistic copy of the amplitude $G_{N-i_1, J}(q)$. Similarly, the amplitude denoted by $G_{N-j_1, I}(q)$ is associated with the $N - j_1$ atoms of the configuration \mathcal{C}_J numbered from $j_1 + 1$ to N . It is a probabilistic copy of the amplitude $G_{N-j_1, I}(q)$.

Let us introduce the generating series

$$\begin{aligned}\Gamma_I(z, q) &= \sum_{N \geq 1} \sum_{\mathcal{C}_{N,I}} G_{N,I}(q) z^N, \\ \Gamma_J(z, q) &= \sum_{N \geq 1} \sum_{\mathcal{C}_{N,J}} G_{N,J}(q) z^N, \\ \Gamma(z, q) &= \Gamma_I(z, q) + \Gamma_J(z, q).\end{aligned}\tag{3.8}$$

The renewal equations (3.6) entail that these quantities obey

$$\begin{aligned}\Gamma_I(z, q) &= \gamma(z, q) + I(ze^{-iq})\Gamma_J(z, q), \\ \Gamma_J(z, q) &= J(ze^{-iq})\Gamma_I(z, q),\end{aligned}\tag{3.9}$$

with

$$\gamma(z, q) = \frac{e^{-iq}}{1 - e^{-iq}} (I(z) - I(ze^{-iq})) (1 + \mathcal{N}_J(z)).\tag{3.10}$$

Solving the linear equations (3.9), we obtain

$$\begin{aligned}\Gamma_I(z, q) &= \frac{\gamma(z, q)}{1 - I(ze^{-iq})J(ze^{-iq})}, \\ \Gamma_J(z, q) &= \frac{J(ze^{-iq})\gamma(z, q)}{1 - I(ze^{-iq})J(ze^{-iq})}, \\ \Gamma(z, q) &= \frac{(1 + J(ze^{-iq}))\gamma(z, q)}{1 - I(ze^{-iq})J(ze^{-iq})}.\end{aligned}\tag{3.11}$$

In the limit of an infinitely long sample, in line with (2.15), the mean Fourier amplitude is given by

$$\langle G(q) \rangle = \lim_{z \rightarrow z_*} \frac{\Gamma(z, q)}{\mathcal{N}(z)}.\tag{3.12}$$

Using (2.9), (3.10) and (3.11), we are left with

$$\langle G(q) \rangle = \frac{e^{-iq}}{1 - e^{-iq}} \frac{1 + J(z_* e^{-iq})}{1 + I(z_*)} \frac{I(z_*) - I(z_* e^{-iq})}{1 - I(z_* e^{-iq})J(z_* e^{-iq})}.\tag{3.13}$$

This result diverges at small wavevectors as

$$\langle G(q) \rangle \approx \frac{\rho}{iq} \quad (q \rightarrow 0),\tag{3.14}$$

where the particle density ρ is given by (2.26).

3.3. Structure factor

The structure factor $S(q)$ encodes bulk properties of the model. Boundary conditions are therefore irrelevant, so that it is sufficient to consider configurations of type \mathcal{C}_I . The simplest route to evaluate $S(q)$ consists in eliminating amplitudes of the form $G_{N,J}(q)$ from the renewal equations (3.6), obtaining thus

$$G_{N,I}(q) = a(i_1, q) + e^{-iq(i_1+j_1)} G_{N-i_1-j_1, I}(q),\tag{3.15}$$

with the same convention as in (3.6), and so

$$\begin{aligned}G_{N,I}(q)\overline{G}_{N,I}(q) &= a(i_1, q)\overline{a}(i_1, q) \\ &\quad + a(i_1, q)e^{iq(i_1+j_1)}\overline{G}_{N-i_1-j_1, I}(q) \\ &\quad + \overline{a}(i_1, q)e^{-iq(i_1+j_1)}G_{N-i_1-j_1, I}(q) \\ &\quad + G_{N-i_1-j_1, I}(q)\overline{G}_{N-i_1-j_1, I}(q).\end{aligned}\tag{3.16}$$

Here and throughout the following, a bar denotes complex conjugation.

Let us introduce the generating series

$$\Sigma(z, q) = \sum_{N \geq 1} \sum_{\mathcal{C}_{N,I}} G_{N,I}(q) \overline{G}_{N,I}(q) z^N. \quad (3.17)$$

This quantity is given by the sum of four terms, in correspondence with the four lines of the right-hand side of (3.16), namely

$$\begin{aligned} \Sigma_1(z, q) &= \frac{2I(z) - I(ze^{iq}) - I(ze^{-iq})}{2(1 - \cos q)} (1 + \mathcal{N}_J(z)), \\ \Sigma_2(z, q) &= \frac{e^{-iq}}{1 - e^{-iq}} (I(ze^{iq}) - I(z)) J(ze^{iq}) \overline{\Gamma}_I(z, q), \\ \Sigma_3(z, q) &= \frac{e^{iq}}{1 - e^{iq}} (I(ze^{-iq}) - I(z)) J(ze^{-iq}) \Gamma_I(z, q), \\ \Sigma_4(z, q) &= I(z) J(z) \Sigma(z, q). \end{aligned} \quad (3.18)$$

We have therefore

$$\Sigma(z, q) = \frac{\Sigma_1(z, q) + \Sigma_2(z, q) + \Sigma_3(z, q)}{1 - I(z) J(z)}. \quad (3.19)$$

In the limit of an infinitely long sample, in line with (2.15), the structure factor is given by

$$S(q) = \lim_{z \rightarrow z_*} \frac{\Sigma(z, q)}{z \mathcal{N}'_I(z)}, \quad (3.20)$$

where the denominator

$$z \mathcal{N}'_I(z) = \sum_{N \geq 1} N \mathcal{N}_{N,I} z^N \quad (3.21)$$

takes care of the factor N in the definition (3.3) of $S_N(q)$. This quantity has a double pole at $z = z_*$, of the form

$$z \mathcal{N}'_I(z) \approx \frac{\ell I(z_*) (1 + J(z_*))}{(1 - I(z) J(z))^2}, \quad (3.22)$$

where the length ℓ is given by (2.25).

Some algebra using (3.18), (3.19), (3.22) leads us to the following expression for the structure factor:

$$S(q) = \frac{\Phi(e^{iq}) + \Phi(e^{-iq})}{2\ell(1 - \cos q)}, \quad (3.23)$$

with

$$\Phi(e^{iq}) = \frac{(I(z_*) - I(z_* e^{iq}))(J(z_*) - J(z_* e^{iq}))}{1 - I(z_* e^{iq}) J(z_* e^{iq})}. \quad (3.24)$$

The formula (3.23) is the key result of this work. First of all, this expression is invariant under the interchange of particles and holes, as it should be. For all models in the rational class under consideration, the structure factor $S(q)$ can be reduced to a rational function of $\cos q$. Numerous explicit examples will be given hereafter (see (4.4), (4.10), (4.15), (5.7), (5.11), (6.6), (6.10)). Its denominator is a polynomial in $\cos q$ whose degree is generically $\Delta - 1$, where Δ is the degree of the polynomial $D(z)$

introduced in (2.13). The structure factor has poles at the complex values $\pm q_m$ of the wavevector, such that

$$e^{iq_m} = \frac{z_\star}{z_m}, \quad (3.25)$$

where the z_m are the zeros of $D(z)$, except the smallest one z_\star . There are $\Delta - 1$ such zeros, counted with their multiplicities. The z_m are either real, or they occur in complex conjugate pairs. They are assumed to be ordered such that

$$z_\star < |z_1| \leq |z_2| \leq \dots, \quad 0 < \text{Im } q_1 \leq \text{Im } q_2 \leq \dots \quad (3.26)$$

The structure factor at zero wavevector,

$$S(0) = \sum_{n=-\infty}^{\infty} C_n, \quad (3.27)$$

is nothing but the compressibility of the model. This quantity describes the linear growth of the variance of the total particle number,

$$M = \sum_{m=1}^N \eta_m, \quad (3.28)$$

in a finite system of size N :

$$\text{var } M = \langle M^2 \rangle - \langle M \rangle^2 \approx S(0) N. \quad (3.29)$$

Expanding (3.23) in q , and using (2.24) and (2.28), we obtain

$$S(0) = \frac{\langle j \rangle^2 (\langle i^2 \rangle - \langle i \rangle^2) + \langle i \rangle^2 (\langle j^2 \rangle - \langle j \rangle^2)}{\ell^3}. \quad (3.30)$$

An equivalent formula was derived by another route in [44], where $S(0)$ is denoted by c_2 .

The structure factor at wavevector π ,

$$S(\pi) = \sum_{n=-\infty}^{\infty} (-1)^n C_n, \quad (3.31)$$

can be referred to as the staggered compressibility. It reads

$$S(\pi) = \frac{(I(z_\star) - I(-z_\star))(J(z_\star) - J(-z_\star))}{2\ell(1 - I(-z_\star)J(-z_\star))}. \quad (3.32)$$

The structure factor exhibits systematic extinctions in cases where the lengths of all clusters of particles (or of holes) are multiples of some fixed integer $K = 2, 3, \dots$. This phenomenon is to be expected. Consider for definiteness the case of particle clusters. If all their lengths are multiples of K , $I(z)$ is a rational function of z^K , so that the expression (3.23) of $S(q)$ vanishes whenever $e^{iqK} = 1$, but $e^{iq} \neq 1$, i.e., for all wavevectors of the form

$$q = \frac{2\pi m}{K} \quad (m \neq 0 \text{ mod } K). \quad (3.33)$$

In the particular case of a symmetric ensemble, where particles and holes play similar roles, such that $\mathcal{I} = \mathcal{J}$, $I(z_\star) = J(z_\star) = 1$, and $\rho = 1/2$, (3.23) and (3.30) boil down to

$$S(q) = \frac{1}{\ell(1 - \cos q)} \frac{1 - I(z_\star e^{iq})I(z_\star e^{-iq})}{(1 + I(z_\star e^{iq}))(1 + I(z_\star e^{-iq}))}, \quad (3.34)$$

$$S(0) = \frac{\langle i^2 \rangle - \langle i \rangle^2}{4\langle i \rangle}. \quad (3.35)$$

The above expressions bear a striking resemblance with those of the Hendricks-Teller model (see (A.11), (A.13)).

3.4. Correlation function

The correlation function is given by (see (3.5))

$$C_n = \int_0^{2\pi} \frac{dq}{2\pi} e^{inq} S(q). \quad (3.36)$$

Setting $y = e^{iq}$ and using (3.23), this reads

$$C_n = -\frac{1}{\ell} \oint \frac{dy}{2\pi i} \frac{y^n}{(y-1)^2} (\Phi(y) + \Phi(1/y)). \quad (3.37)$$

The integration contour in (3.37) is the unit circle, along which the integrand is regular. The differential element $dy/(y-1)^2$ is invariant if y is changed into $1/y$. This ensures the expected symmetry $C_n = C_{-n}$.

Henceforth we consider $n \geq 0$ for definiteness. The integral in (3.37) receives contributions from the poles of $\Phi(1/y)$ at $y_m = e^{iq_m} = z_*/z_m$ (see (3.25)).

Let us assume for a while that all the zeros z_m are simple and that $\Phi(\infty)$ is finite. In this situation, the correlation function is a finite sum of decaying exponentials:

$$C_n = \sum_{m=1}^{\Delta-1} A_m \left(\frac{z_*}{z_m}\right)^n \quad (n \geq 0), \quad (3.38)$$

with amplitudes

$$A_m = \frac{z_*}{\ell} \frac{2 - I(z_*)J(z_m) - I(z_m)J(z_*)}{(z_* - z_m)^2 (I'(z_m)J(z_m) + I(z_m)J'(z_m))}. \quad (3.39)$$

The correlation therefore decays exponentially with distance, as

$$C_n \sim e^{-n/\xi}, \quad (3.40)$$

where the correlation length reads

$$\xi = \frac{1}{\ln \frac{|z_1|}{z_*}} = \frac{1}{\text{Im } q_1}. \quad (3.41)$$

Let us now relax the two assumptions above. If the zero z_m is not simple, but has multiplicity $m \geq 2$, the corresponding amplitude A_m in (3.38) is replaced by a polynomial in n of degree at most $m-1$. If $\Phi(\infty)$ is not finite, then $\Phi(y)$ grows as y^μ at large y , where μ is some positive integer. As a consequence, the formula (3.38) for C_n might be modified for the first few values of the distance n ($n = 0, \dots, \mu-1$). In all cases, the correlation length is given by (3.41).

The correlation function admits an appealing alternative expression, which holds in full generality. Consider the function $\Phi(e^{iq})$ defined in (3.24). This function equals unity in the limit $e^{iq} \rightarrow 0$, whereas it vanishes for $q \rightarrow 0$ as

$$\Phi(e^{iq}) \approx -iqR, \quad (3.42)$$

with

$$R = \frac{z_* I'(z_*) J'(z_*)}{I'(z_*) J(z_*) + I(z_*) J'(z_*)} = \frac{\langle i \rangle \langle j \rangle}{\ell} = \rho(1 - \rho)\ell. \quad (3.43)$$

Moreover, the function $\Phi(e^{iq})$ is regular at least for $|e^{iq}| < 1$. Its poles are indeed situated at e^{-iq_m} (see (3.25)). It can therefore be expanded as

$$\Phi(e^{iq}) = \sum_{a=1}^{\infty} r_a (1 - e^{iaq}). \quad (3.44)$$

The amplitudes r_a are real, but not positive in general. They obey the sum rules

$$\sum_{a=1}^{\infty} r_a = 1, \quad \sum_{a=1}^{\infty} ar_a = R. \quad (3.45)$$

Moreover, the rational expression (3.24) of $\Phi(e^{iq})$ implies that the amplitudes r_a obey a linear recursion of the form

$$\lambda_0 r_a + \lambda_1 r_{a+1} + \lambda_2 r_{a+2} + \dots = 0, \quad (3.46)$$

except for finitely many initial values of a . The number of terms involved in this recursion is generically Δ , the degree of the polynomial $D(z)$ introduced in (2.13). The coefficients $\lambda_0, \lambda_1, \lambda_2 \dots$ are constants dictated by the model.

In terms of the amplitudes r_a , the formula (3.23) for the structure factor reads

$$S(q) = \frac{1}{\ell} \sum_{a=1}^{\infty} r_a \frac{1 - \cos aq}{1 - \cos q}. \quad (3.47)$$

Inserting this expression into (3.36), we obtain

$$C_n = \frac{1}{\ell} \sum_{a=1}^{\infty} r_a I_{a,n}, \quad (3.48)$$

with

$$I_{a,n} = \int_0^{2\pi} \frac{dq}{2\pi} e^{inq} \frac{1 - \cos aq}{1 - \cos q} = \begin{cases} a - |n| & (a > |n|), \\ 0 & (a \leq |n|). \end{cases} \quad (3.49)$$

Let us henceforth consider $n \geq 0$. The correlation function has the following expression in terms of the amplitudes r_a :

$$C_n = \frac{1}{\ell} \sum_{a=n+1}^{\infty} (a - n)r_a. \quad (3.50)$$

Using (3.43) and (3.45), this formula can be recast as

$$C_n = \rho(1 - \rho) - \frac{1}{\ell} \left(n - \sum_{a=1}^{n-1} (n - a)r_a \right). \quad (3.51)$$

The correlation function therefore obeys the three-term recursion

$$2C_n - C_{n-1} - C_{n+1} = -\frac{r_n}{\ell} \quad (n \geq 1). \quad (3.52)$$

As a consequence, the C_n also obey the linear recursion relation (3.46), i.e.,

$$\lambda_0 C_n + \lambda_1 C_{n+1} + \lambda_2 C_{n+2} + \dots = 0, \quad (3.53)$$

except for finitely many initial values of n , and C_n and r_n share the same exponential decay (3.40).

The expression (3.51) yields in particular

$$C_0 = \rho(1 - \rho), \quad C_1 = \rho(1 - \rho) - \frac{1}{\ell}. \quad (3.54)$$

These two results are expected. The first one is obvious from the definition of C_0 . The second one expresses that the densities of $\bullet\circ$ and $\circ\bullet$ cluster interfaces have the expected value, namely

$$\lim_{m \rightarrow \infty} \langle \eta_m (1 - \eta_{m+1}) \rangle = \rho - \rho^2 - C_1 = \frac{1}{\ell}. \quad (3.55)$$

At larger distances ($n \geq 2$), the correlation function is not universal, in the sense that it depends on the individual amplitudes r_a . We have

$$C_2 = \rho(1 - \rho) - \frac{2 - r_1}{\ell}, \quad C_3 = \rho(1 - \rho) - \frac{3 - 2r_1 - r_2}{\ell}, \quad (3.56)$$

and so on.

4. Three simple examples

In this section we illustrate the above general results on the structure factor $S(q)$ and on the correlation function C_n by considering three simple examples of statistical ensembles, already studied in [44], which virtually exhaust all cases with $\Delta = 1$ or $\Delta = 2$.

4.1. Flat ensemble

The simplest statistical ensemble of all is the flat one, where all cluster lengths are permitted. This corresponds to $\mathcal{I} = \mathcal{J} = \{1, 2, 3, \dots\}$, hence

$$I(z) = J(z) = \frac{z}{1 - z}, \quad (4.1)$$

so that

$$D(z) = 1 - 2z, \quad (4.2)$$

and so $\Delta = 1$. We have

$$z_\star = \frac{1}{2}, \quad \rho = \frac{1}{2}, \quad \ell = 4. \quad (4.3)$$

Equation (3.23) reads

$$S(q) = \frac{1}{4}, \quad (4.4)$$

and so

$$C_n = \frac{\delta_{n0}}{4}, \quad (4.5)$$

where δ_{ab} is the Kronecker symbol.

The absence of correlations between the occupancies of different sites reflects the property that each site of the lattice is independently either occupied or empty. Concomitantly, the sum entering (3.38) is empty for $\Delta = 1$.

4.2. Isolated empty sites

Our second example is defined by the condition that empty sites (i.e., holes) are isolated. The ensemble where occupied sites (i.e., particles) are isolated is related to the present one by exchanging the roles of particles and holes. Both models share the same structure factor and correlation function. These ensembles have been considered in several contexts, including the attractors of repulsion processes [51] and packings of disks in narrow channels [52, 53].

This example corresponds to $\mathcal{I} = \{1, 2, 3, \dots\}$ and $\mathcal{J} = \{1\}$, hence

$$I(z) = \frac{z}{1 - z}, \quad J(z) = z, \quad (4.6)$$

so that

$$D(z) = 1 - z - z^2, \quad (4.7)$$

and so $\Delta = 2$. We have

$$z_* = \frac{\sqrt{5} - 1}{2} \approx 0.618033, \quad (4.8)$$

$$\rho = \frac{5 + \sqrt{5}}{10} \approx 0.723606, \quad \ell = \frac{5 + \sqrt{5}}{2} \approx 3.618033. \quad (4.9)$$

Equation (3.23) reads

$$S(q) = \frac{1}{\sqrt{5}(3 + 2 \cos q)}, \quad (4.10)$$

and so

$$C_n = \frac{1}{5} \left(-\frac{3 - \sqrt{5}}{2} \right)^n \quad (n \geq 0). \quad (4.11)$$

The correlation function is a pure decaying exponential, in agreement with (3.38) for $\Delta = 2$.

4.3. Even particle clusters

Our third example is defined by the condition that clusters of particles have even lengths. This corresponds to $\mathcal{I} = \{2, 4, 6, \dots\}$ and $\mathcal{J} = \{1, 2, 3, \dots\}$, i.e.,

$$I(z) = \frac{z^2}{1 - z^2}, \quad J(z) = \frac{z}{1 - z}. \quad (4.12)$$

Here again,

$$D(z) = 1 - z - z^2 \quad (4.13)$$

and $\Delta = 2$, so that z_* is given by (4.8). We have

$$\rho = \frac{5 - \sqrt{5}}{5} \approx 0.552786, \quad \ell = \frac{5 + 3\sqrt{5}}{2} \approx 5.854101. \quad (4.14)$$

Equation (3.23) reads

$$S(q) = \frac{2(1 + \cos q)}{\sqrt{5}(3 + 2 \cos q)}. \quad (4.15)$$

The structure factor vanishes for $q = \pi$. This is an extinction of the form (3.33) with $K = 2$. The correlation function reads

$$C_n = \frac{\delta_{n0}}{\sqrt{5}} - \frac{1}{5} \left(-\frac{3 - \sqrt{5}}{2} \right)^n \quad (n \geq 0). \quad (4.16)$$

The expression for $n = 0$ is modified with respect to the decaying exponential (3.38). This is an instance of the situation described below (3.41), with $\mu = 1$.

Figure 1 shows plots of the structure factor $S(q)$ against q/π for the three ensembles investigated in this section.

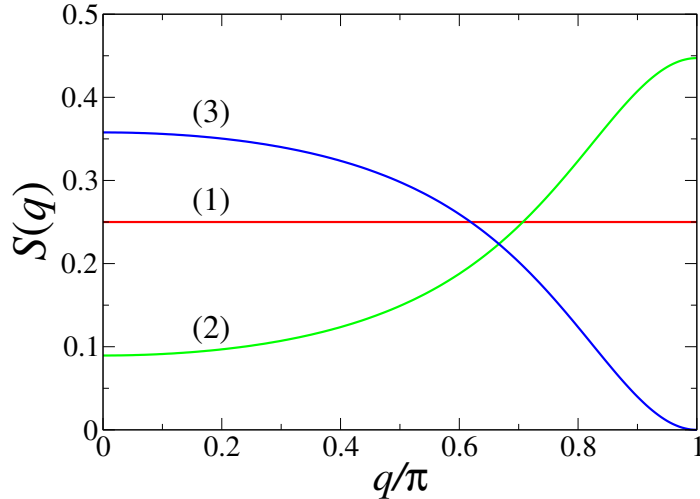


Figure 1. Structure factor $S(q)$ of the three ensembles investigated in section 4, plotted against q/π . Red curve (1): flat ensemble (see (4.4)). Green curve (2): isolated empty sites (see (4.10)). Blue curve (3): even particle clusters (see (4.15)).

5. The k -mer deposition model

The sequential deposition of k -mers is a fully irreversible process where k -mers (clusters of k particles) are deposited at random positions on an initially empty one-dimensional lattice. The process stops when the system reaches a blocked (or jammed) configuration where no further k -mer can be inserted any more [54, 55, 56]. The integer $k \geq 2$ is the only parameter of the model. The sequential deposition of dimers ($k = 2$) is equivalent to a dimerization model investigated long ago by Flory [57].

The statistical ensemble of blocked configurations of k -mers has been studied by various approaches [41, 42, 34, 44, 43]. In [44] it has been shown that this ensemble can be described in terms of independent clusters, and therefore studied within the present renewal formalism, with $\mathcal{I} = \{k, 2k, 3k, \dots\}$ and $\mathcal{J} = \{1, 2, \dots, k-1\}$, so that

$$I(z) = \frac{z^k}{1 - z^k}, \quad J(z) = \frac{z - z^k}{1 - z}. \quad (5.1)$$

The polynomial $D(z)$ can be reduced to

$$D(z) = 1 - (z^k + z^{k+1} + \dots + z^{2k-1}), \quad (5.2)$$

and so

$$\Delta = 2k - 1. \quad (5.3)$$

For all values of the integer k , the structure factor is expected to exhibit systematic extinctions at wavevectors that are multiples of $2\pi/k$ (see (3.33)).

5.1. The first few values of k

It is interesting to start by considering the first few values of k , where closed-form formulas can be derived.

Dimers ($k = 2$). This case is the simplest of all. We have

$$D(z) = 1 - z^2 - z^3, \quad (5.4)$$

and so $\Delta = 3$. We thus recover that

$$z_\star = \frac{1}{6} \left((100 + 12\sqrt{69})^{1/3} + (100 - 12\sqrt{69})^{1/3} - 2 \right) \approx 0.754877 \quad (5.5)$$

is the reciprocal of the so-called plastic number [44], whereas

$$\rho = \frac{2(7 + 2z_\star + 3z_\star^2)}{23} \approx 0.822991. \quad (5.6)$$

Even in this simple case, (3.23) yields a rather lengthy expression for the structure factor. Repeated use of $D(z_\star) = 0$ reduces this expression to a minimal form where the highest power of z_\star is $\Delta - 1$ (here, 2). We shall do this reduction throughout the following. We thus obtain

$$S(q) = \frac{2z_\star(1 - z_\star)(1 + \cos q)}{A_2(\cos q)}, \quad (5.7)$$

with

$$\begin{aligned} A_2(\cos q) &= 3 - z_\star^2 - 2(4 - 5z_\star - 5z_\star^2) \cos q \\ &\quad - 4(3 - 2z_\star - 4z_\star^2) \cos^2 q. \end{aligned} \quad (5.8)$$

The extinction at $q = \pi$ is clearly visible on (5.7).

Trimers ($k = 3$). In this case we have $\Delta = 5$, but $D(z)$ factors as

$$D(z) = (1 + z^2)(1 - z^2 - z^3), \quad (5.9)$$

so that z_\star is again given by (5.5), whereas

$$\rho = \frac{3(26 + 7z_\star - 2z_\star^2)}{115} \approx 0.786377. \quad (5.10)$$

Equation (3.23) yields

$$S(q) = \frac{(1 + 2(1 - z_\star) \cos q)(1 + 2 \cos q)^2}{A_3(\cos q)}, \quad (5.11)$$

with

$$\begin{aligned} A_3(\cos q) &= -(1 - 2z_\star)(2 + 3z_\star) + 2(9 + z_\star - 13z_\star^2) \cos q \\ &\quad + 4(4 - 3z_\star)(2 + 3z_\star) \cos^2 q - 8(3 - 6z_\star - 10z_\star^2) \cos^3 q \\ &\quad - 16(1 - 2z_\star)(2 + 3z_\star) \cos^4 q. \end{aligned} \quad (5.12)$$

The extinction at $q = 2\pi/3$ is clearly visible on (5.11).

The formulas (5.7) and (5.11) show that the complexity of the analytical expression of $S(q)$ increases fast with the integer k . The structure factor indeed exhibits more and more detailed structures as k increases, as testified by figure 2.

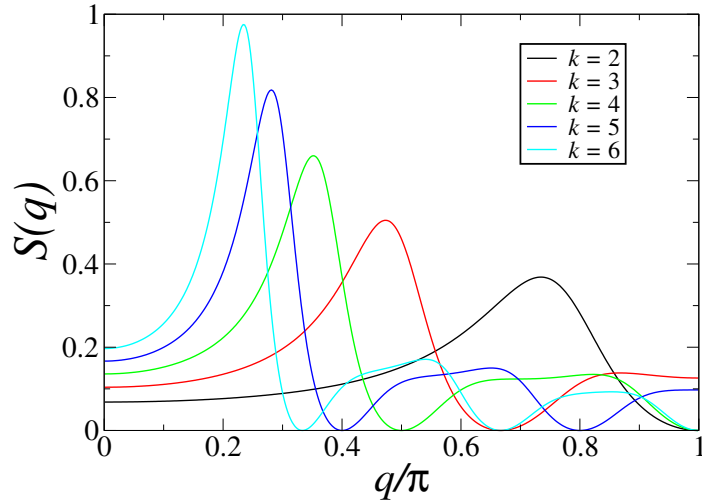


Figure 2. Structure factor $S(q)$ of the k -mer deposition model, plotted against q/π , for k ranging from 2 to 6 (see legend).

5.2. Scaling behavior at large k

Static observables of the k -mer deposition model have been shown in [44] to exhibit an unusual behavior at large k , where logarithmic corrections to scaling are ubiquitous. These corrections to scaling already show up in z_* . Setting

$$z_* = \exp\left(-\frac{u_*}{k}\right), \quad (5.13)$$

we find that u_* obeys the transcendental equation

$$u_* e^{u_*} \approx k. \quad (5.14)$$

This equation holds up to corrections of relative order $1/k$, which will be consistently neglected throughout the following. The solution to (5.14) reads

$$u_* \approx W(k), \quad (5.15)$$

in terms of the Lambert W function. To leading order, this reads

$$u_* \approx \ln k. \quad (5.16)$$

More precisely, setting

$$\lambda = \ln k, \quad \mu = \ln \lambda = \ln \ln k, \quad (5.17)$$

we obtain the full asymptotic series

$$u_* = \lambda - \mu + \frac{\mu}{\lambda} + \frac{\mu(\mu-2)}{2\lambda^2} + \frac{\mu(2\mu^2-9\mu+6)}{6\lambda^3} + \dots \quad (5.18)$$

The main outcomes of the scaling analysis performed in [44] which are relevant for the present purpose are as follows:

$$\rho \approx \frac{u_*}{u_*+1}, \quad \ell \approx \frac{u_*+1}{u_*} k. \quad (5.19)$$

The scaling analysis recalled above can be extended to the structure factor all over its scaling regime where q scales as the inverse of k . Introducing the rescaled wavevector

$$Q = kq, \quad (5.20)$$

we have the estimates

$$\begin{aligned} I(z_\star) &\approx \frac{u_\star}{k}, & I(z_\star e^{\pm iq}) &\approx \frac{u_\star e^{\pm iQ}}{k}, \\ J(z_\star) &\approx \frac{k}{u_\star}, & J(z_\star e^{\pm iq}) &\approx \frac{k}{u_\star \mp iQ}, \end{aligned} \quad (5.21)$$

so that (3.23) evaluates to

$$S(q) \approx k \frac{u_\star}{u_\star + 1} \frac{2(1 - \cos Q)}{2u_\star^2(1 - \cos Q) + 2u_\star Q \sin Q + Q^2}. \quad (5.22)$$

The second factor of this expression is equal to the particle density ρ (see (5.19)). The third factor mainly depends on the rescaled wavevector Q . The presence of powers of u_\star however generates logarithmic corrections to this main scaling behavior. We have in particular

$$S(0) \approx \frac{ku_\star}{(u_\star + 1)^3}. \quad (5.23)$$

An equivalent formula was derived by another route in [44]. The expression

$$C_0 = \rho(1 - \rho) \approx \frac{u_\star}{(u_\star + 1)^2} \quad (5.24)$$

translates to the non-trivial identity

$$\int_{-\infty}^{\infty} dQ \frac{1 - \cos Q}{2u_\star^2(1 - \cos Q) + 2u_\star Q \sin Q + Q^2} = \frac{\pi}{u_\star + 1}. \quad (5.25)$$

The scaling form (5.22), with its fast decay in $1/Q^2$, corroborates the most salient feature of figure 2, namely that most of the intensity concentrates onto smaller and smaller values of q as k is increased.

Let us focus our attention onto the leading peak of the structure factor, located slightly before the first extinction at $q = 2\pi/k$, whose height grows rather fast with k . The scaling behavior of the position $Q_{\max} = kq_{\max}$ of this peak and of its height S_{\max} can be extracted from the scaling result (5.22). The peak position obeys the transcendental equation

$$u_\star = \frac{Q_{\max}(2(1 - \cos Q_{\max}) - Q_{\max} \sin Q_{\max})}{2(1 - \cos Q_{\max})(Q_{\max} - \sin Q_{\max})}. \quad (5.26)$$

Some algebra yields the following asymptotic series in inverse powers of u_\star :

$$Q_{\max} = 2\pi \left(1 - \frac{1}{u_\star} + \frac{1}{u_\star^2} + \frac{\pi^2 - 3}{3u_\star^3} + \dots \right), \quad (5.27)$$

$$S_{\max} = \frac{k}{\pi^2} \left(1 + \frac{1}{u_\star} - \frac{2\pi^2}{3u_\star^3} + \dots \right). \quad (5.28)$$

The peak height S_{\max} therefore grows linearly with k , i.e., faster than $S(0) \approx k/(\ln k)^2$ (see (5.23)) by a factor growing as $(\ln k)^2$. This is illustrated in figure 3, showing plots of $S(0)$ and S_{\max} against k . Dashed lines with corresponding colors show appropriate approximations (see caption).

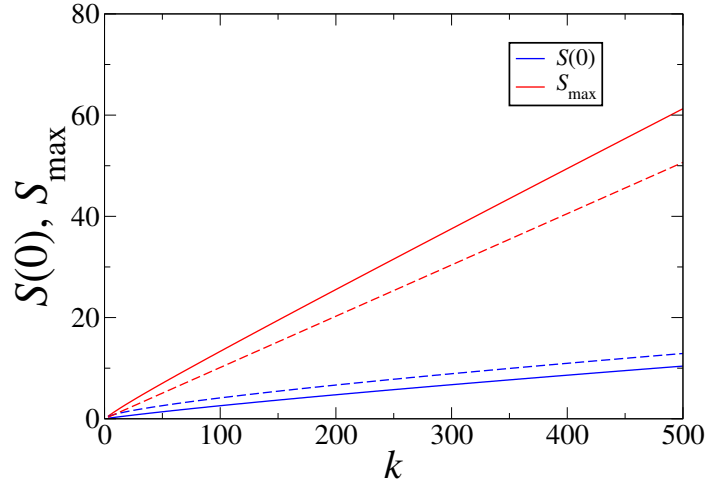


Figure 3. Plots of $S(0)$ and S_{\max} against k , for the k -mer deposition model. Full blue curve: exact values of $S(0)$ for finite k (see (3.30)). Dashed blue curve: scaling prediction (see (5.13), (5.23)). Full red curve: numerically exact maximal values of $S(q)$ for finite k . Dashed red curve: leading linear growth in k/π^2 (see (5.28)).

The peak position Q_{\max} is very near the first pair of complex poles of the structure factor, i.e., $Q_1 = kq_1$ and $\bar{Q}_1 = k\bar{q}_1$, where

$$Q_1 = 2\pi \left(1 - \frac{1}{u_*} + \frac{1 + i\pi}{u_*^2} - \frac{4\pi^2 + 3 + 9i\pi}{3u_*^3} + \dots \right). \quad (5.29)$$

Taking the imaginary part of this expression to leading order in $1/u_*$ and using (3.41), we obtain that the correlation length scales as

$$\xi \approx \frac{ku_*^2}{2\pi^2} \approx \frac{k(\ln k)^2}{2\pi^2}. \quad (5.30)$$

6. Arrays of Rydberg atoms

This section is devoted to blocked configurations of arrays of Rydberg atoms on a one-dimensional optical lattice. We consider the simple setting recalled in section 1, where each lattice site occupied by a Rydberg atom must have at least b empty sites on either side. The integer $b \geq 1$, referred to as the blockade range, is the only parameter of the model.

Our aim is to investigate the uniform ensemble of all blocked configurations, where no further atom can be inserted into the system. Along the lines of earlier works [34, 43, 44], blocked configurations consist of isolated occupied sites (the Rydberg atoms) separated by clusters of holes whose length is at least b , in order to obey the blockade constraint, and at most $2b$, since an extra Rydberg atom could be inserted in the middle of an empty range of size $2b + 1$.

Within the present formalism, clusters of particles and of holes respectively correspond to $\mathcal{I} = \{1\}$ and $\mathcal{J} = \{b, b + 1, \dots, 2b\}$, and so

$$I(z) = z, \quad J(z) = \frac{z^b(1 - z^{b+1})}{1 - z}. \quad (6.1)$$

The polynomial $D(z)$ can be reduced to

$$D(z) = 1 - (z^{b+1} + z^{b+2} + \dots + z^{2b+1}). \quad (6.2)$$

This expression coincides with (5.2), with the identification

$$k = b + 1. \quad (6.3)$$

We have in particular

$$\Delta = 2b + 1. \quad (6.4)$$

There is indeed an equivalence, at the level of single configurations, between blocked configurations of k -mers and of Rydberg atoms. A Rydberg atom followed by b empty sites (to its right) can be mapped onto a k -mer, where b and k are related by (6.3). The mapping between configurations of k -mers and of Rydberg atoms is however not unique [43, 44]. Many observables pertaining to both models are simply related to each other. For instance, the density of the k -mer deposition model is k times larger than the corresponding density of Rydberg atoms.

As a consequence of the above correspondence, the structure factors of k -mers and Rydberg atoms with $b = k - 1$ share the same denominator. The latter is indeed a polynomial in $\cos q$ that is essentially dictated by $D(z)$. Both structure factors have different numerators, if only because there are no extinctions in the case of Rydberg atoms.

6.1. The first few values of b

It is again interesting to first look at a few smallest values of the blockade range b .

$b = 1$. This case is the simplest of all. It corresponds to $k = 2$, so that (5.4) and (5.5) still hold, whereas

$$\rho = \frac{7 + 2z_\star + 3z_\star^2}{23} \approx 0.411495. \quad (6.5)$$

Equation (3.23) yields

$$S(q) = \frac{1}{B_1(\cos q)}, \quad (6.6)$$

with

$$\begin{aligned} B_1(\cos q) &= 5 + 7z_\star + 5z_\star^2 + 2(7 + 8z_\star + 2z_\star^2) \cos q \\ &\quad + 4(2 + 3z_\star) \cos^2 q. \end{aligned} \quad (6.7)$$

We have (see (5.8))

$$B_1(\cos q) = (2 + 3z_\star + 2z_\star^2)A_2(\cos q). \quad (6.8)$$

It is indeed expected from the correspondence between k -mers and Rydberg atoms that the denominators of (5.7) and (6.6) should coincide, up to some q -independent multiplicative constant.

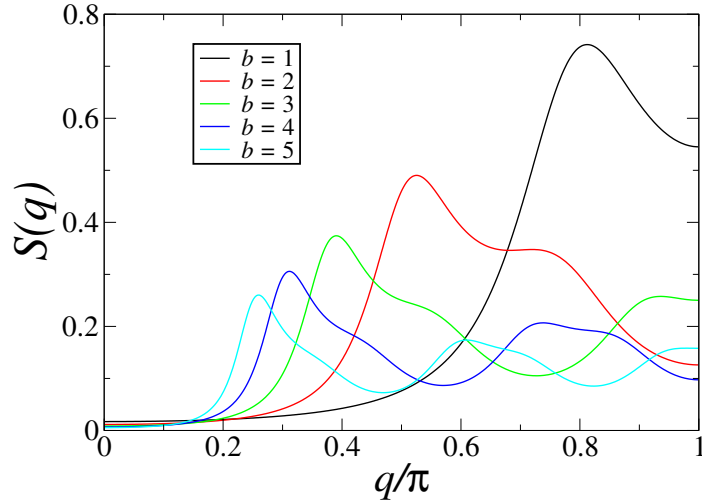


Figure 4. Structure factor $S(q)$ of the blocked arrays of Rydberg atoms, plotted against q/π , for blockade ranges b running from 1 to 5 (see legend).

$b = 2$. This case corresponds to $k = 3$, so that (5.5) and (5.9) still hold, whereas

$$\rho = \frac{26 + 7z_* - 2z_*^2}{115} \approx 0.262125. \quad (6.9)$$

Equation (3.23) yields

$$S(q) = \frac{(1 + z_*)^2 + 2z_* \cos q}{B_2(\cos q)}, \quad (6.10)$$

with

$$\begin{aligned} B_2(\cos q) = & 5 + 3z_* - z_*^2 - 2(3 - 6z_* - 10z_*^2) \cos q \\ & + 4(5 + 13z_* + 14z_*^2) \cos^2 q + 8(13 + 10z_* + 3z_*^2) \cos^3 q \\ & + 16(5 + 3z_* - z_*^2) \cos^4 q. \end{aligned} \quad (6.11)$$

We have (see (5.12))

$$B_2(\cos q) = (1 + z_*)^2 A_3(\cos q). \quad (6.12)$$

A relationship of this kind was again expected from the correspondence between k -mers and Rydberg atoms.

Equations (6.6) and (6.10) demonstrate that the complexity of the structure factor increases fast with the blockade range b . Concomitantly, $S(q)$ exhibits more and more detailed structures as b increases (see figure 4).

6.2. Scaling behavior at large b

The scaling analysis of the k -mer deposition model at large k summarized in section 5.2 applies, mutatis mutandis, to the blocked configurations of Rydberg atoms in the regime where the blockade range b becomes large [44]. Here, too, logarithmic corrections to scaling are ubiquitous. Setting

$$z_* = \exp\left(-\frac{u_*}{b}\right), \quad (6.13)$$

we find that u_* again obeys the transcendental equation (5.14), and we have

$$\rho \approx \frac{u_*}{b(u_* + 1)}, \quad \ell \approx \frac{u_* + 1}{u_*} b. \quad (6.14)$$

The scaling analysis again extends to the structure factor all over the regime where q scales as the inverse of the blockade range b . Introducing the rescaled wavevector

$$Q = bq, \quad (6.15)$$

and skipping every detail, we find that (3.23) translates to

$$S(q) \approx \frac{u_*}{b(u_* + 1)} \frac{Q^2}{2u_*^2(1 - \cos Q) + 2u_*Q \sin Q + Q^2}. \quad (6.16)$$

The first factor is equal to the density ρ of Rydberg atoms (see (6.14)). The second factor mainly depends on the rescaled wavevector Q . The denominators of (5.22) and (6.16) coincide, as expected from the correspondence recalled above between k -mers and Rydberg atoms. The numerators are however different. The presence of powers of u_* in (6.16) again generates logarithmic corrections of various kinds. We have in particular

$$S(0) \approx \frac{u_*}{b(u_* + 1)^3}. \quad (6.17)$$

The correlation length is again described by the scaling form (5.30), up to the replacement of k by b , i.e.,

$$\xi \approx \frac{bu_*^2}{2\pi^2} \approx \frac{b(\ln b)^2}{2\pi^2}. \quad (6.18)$$

At variance with the scaling form (5.22), which falls off as $1/Q^2$ for Q large, the expression (6.16) predicts that

$$S(q) \approx \rho \quad (6.19)$$

is roughly constant and equal to the density of Rydberg atoms for $|Q| \gg 1/b$, i.e., in practice, for b large and $|q| \gg 1/b$. This density is larger than $S(0)$ by a factor growing as $(\ln b)^2$. The structure factor exhibits oscillations around ρ virtually all over the range of wavevectors, whose amplitude falls off rather rapidly as the blockade range b is increased (see figure 5). Integrating (6.19) over q yields $C_0 \approx \rho$, in agreement with (3.54) since ρ is small at large b .

7. Discussion

This work follows on from a previous paper in collaboration with Krapivsky [44]. There, we have put forward an alternative approach, inspired from the theory of renewal processes, to study statistical ensembles of constrained configurations of particles on a one-dimensional lattice, and especially to determine their configurational entropies. Here, we demonstrate that a range of observables pertaining to such ensembles, including chiefly their structure factor and correlation function, can also be investigated by means of the renewal approach. It is worth recalling that the scope of this approach is restricted to local constraints which are expressible in terms of the lengths of clusters of occupied and empty sites.

We have emphasized the pivotal importance of the class of rational models, which encompasses all examples considered in this paper, and virtually all situations

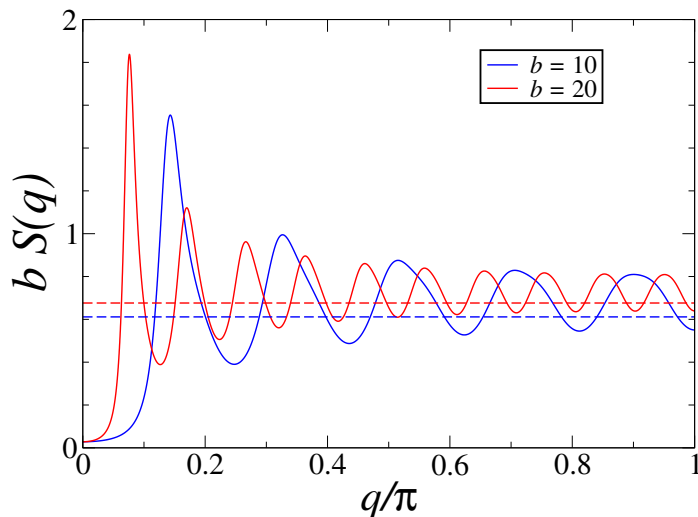


Figure 5. Full lines: structure factor $S(q)$ of Rydberg atoms, multiplied by b and plotted against q/π , for $b = 10$ (blue) and $b = 20$ (red). Dashed lines with corresponding colors: prediction (6.19).

of physical significance. Within this rational class, the complexity of a statistical ensemble is measured by the degree Δ of the polynomial $D(z)$ introduced in (2.13). The integer Δ is fully analogous to the dimension of the transfer matrix in the more traditional transfer-matrix approach. To mention just one example, the decomposition (3.38) of the correlation function as a sum of $\Delta - 1$ decaying exponentials has a perfect analogue in terms of the subleading eigenvalues of the transfer matrix.

To close, we briefly tackle the situation of ensembles of blocked configurations beyond the rational class. To take a striking example, if $\mathcal{I} = \{1, 2, 4, 8, \dots\}$, i.e., the allowed lengths of particle clusters consist of the powers of two, the corresponding generating series

$$I(z) = \sum_{k=0}^{\infty} z^{2^k} \quad (7.1)$$

is a prototypical lacunary series, having the full unit circle of the complex z -plane as a natural boundary. As a consequence, for a generic set \mathcal{J} , the structure factor $S(q)$ has a natural boundary along some curve in the complex q -plane. The structure of the correlation function is therefore exceedingly more complex than the finite sum (3.38). It would be desirable to have even one physically motivated model of this kind.

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Data availability statement

Data sharing not applicable to this article as no datasets were generated or analyzed.

Conflict of interest

The author declares no conflict of interest.

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Appendix A. The Hendricks-Teller model

In this appendix we illustrate the renewal approach used in the body of this paper on a simpler structural model, namely the Hendricks-Teller model [45], defined as follows. Identical pointlike atoms are put along an infinite half-line at random positions x_n such that $x_0 = 0$, and the distances

$$\ell_n = x_n - x_{n-1} \quad (\text{A.1})$$

are independent and identically distributed with some continuous distribution $\rho(\ell)$ such that $\langle \ell^2 \rangle$ is convergent.

The (random) Fourier amplitude $G_N(q)$ and Fourier intensity $S_N(q)$ of the first N atoms read

$$G_N(q) = \sum_{n=1}^N e^{-iqx_n}, \quad S_N(q) = \frac{|G_N(q)|^2}{N}. \quad (\text{A.2})$$

Our main interest is in the structure factor

$$S(q) = \lim_{N \rightarrow \infty} \langle S_N(q) \rangle, \quad (\text{A.3})$$

which is a self-averaging quantity.

The Fourier amplitudes obey the renewal equation

$$G_N(q) = e^{-iq\ell_1} + e^{-iq\ell_1} G_{N-1}(q). \quad (\text{A.4})$$

The mean Fourier amplitude can be derived by averaging (A.4) over the atomic positions. This yields

$$\langle G_N(q) \rangle = g(q) + g(q) \langle G_{N-1}(q) \rangle, \quad (\text{A.5})$$

where

$$g(q) = \int_0^\infty e^{-iq\ell} \rho(\ell) d\ell \quad (\text{A.6})$$

is the Fourier transform of the distribution of interatomic distances. In the limit of an infinitely long sample, the mean amplitude therefore reads

$$\langle G(q) \rangle = \frac{g(q)}{1 - g(q)}. \quad (\text{A.7})$$

This result diverges at small wavevectors as

$$\langle G(q) \rangle \approx \frac{1}{iq \langle \ell \rangle} \quad (q \rightarrow 0). \quad (\text{A.8})$$

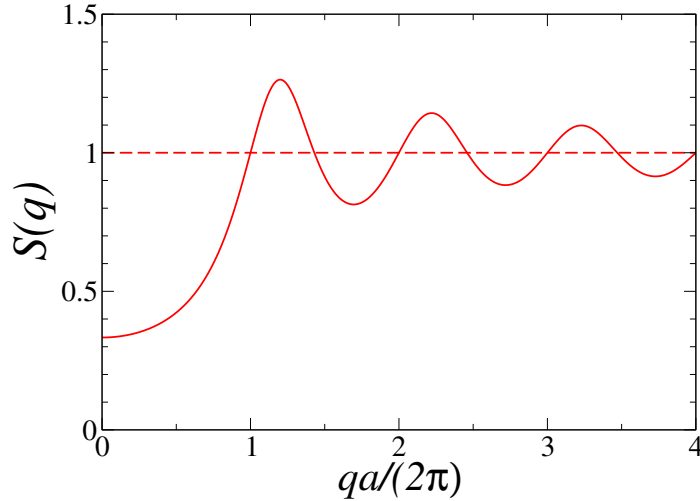


Figure A1. Structure factor (A.14) of the Hendricks-Teller model with a uniform distribution of interatomic distances over the interval $[0, a]$, plotted against $qa/(2\pi)$.

The structure factor can be derived by multiplying (A.4) by its complex conjugate, using (A.2), and averaging over the atomic positions. This yields

$$N\langle S_N(q) \rangle = 1 + \langle G_{N-1}(q) \rangle + \overline{\langle G_{N-1}(q) \rangle} + (N-1)\langle S_{N-1}(q) \rangle. \quad (\text{A.9})$$

In the $N \rightarrow \infty$ limit, the structure factor therefore reads

$$S(q) = 1 + \langle G(q) \rangle + \overline{\langle G(q) \rangle}. \quad (\text{A.10})$$

Using (A.7), we thus recover the main result of [45] for the present model, i.e.,

$$S(q) = \frac{1 - g(q)\overline{g}(q)}{(1 - g(q))(1 - \overline{g}(q))}. \quad (\text{A.11})$$

Let us mention a few properties of the above formula. Whenever the distance distribution $\rho(\ell)$ is continuous, its Fourier transform $g(q)$ falls off to zero at large q , and so the structure factor goes to the limit

$$S(\infty) = 1. \quad (\text{A.12})$$

Its value at $q = 0$,

$$S(0) = \frac{\langle \ell^2 \rangle - \langle \ell \rangle^2}{\langle \ell \rangle^2}, \quad (\text{A.13})$$

is nothing but the reduced variance of interatomic distances. This quantity may be either smaller or larger than unity.

The exponential distance distribution $\rho(\ell) = (1/a)\exp(-\ell/a)$ yields a Poissonian distribution of atoms, for which we have $S(q) = 1$ for all q , as expected.

A simple yet non-trivial example is provided by a uniform distribution of interatomic distances over some interval $[0, a]$. The ensuing structure factor

$$S(q) = \frac{(qa)^2 + 2(\cos qa - 1)}{(qa)^2 + 2(1 - \cos qa - qa \sin qa)} \quad (\text{A.14})$$

is a function of the product qa , starting from $S(0) = 1/3$ and exhibiting slowly damped oscillations with period 2π around its limit $S(\infty) = 1$ (see figure A1).

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