

# **Ensemble Expectations for Structures on Two-Dimensional Lattices**

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Expressions are obtained for the limiting behavior of ensemble expectations, as functions of coverage, of the number of simultaneous occurrences of various structures when indistinguishable single particles are arranged on a two-dimensional lattice. For the general expressions obtained no restrictions are placed on the geometrical nature of the lattice. Averages for specific geometrical arrays, such as rectangular and hexagonal arrays, may be calculated directly from the general results.

## **1. INTRODUCTION**

The treatment of gas–solid adsorption in statistical mechanics requires a consideration of structures on two-dimensional lattices. Specific structures have been examined in previous studies. In the present paper a more general approach is pursued and the following question investigated:

What is the ensemble expectation, as a function of coverage, of the number of simultaneous occurrences of various structures when indistinguishable single particles are distributed on a lattice?

The model assumed for the adsorbent surface is that of a lattice  $\Lambda$  with a fixed number  $N$  of sites. Adsorption occurs as indistinguishable single particles of a classical gas of a single chemical species collide with and are bound to the sites of the lattice. Each site accommodates exactly one adsorbed particle and adsorbate particles are found on the lattice only at the sites.

## **2. ENSEMBLE EXPECTATIONS**

**2.1. Definitions.** A lattice  $\Lambda$  is here taken to be a collection of  $N$  subsets of the usual Cartesian plane. The elements of the collection are called *cells* or *sites*. An *array* is a lattice together with a particular

geometrical arrangement of the sites. For example, an  $R \times Q$  rectangular array is a lattice of cardinality  $N = RQ$  whose elements are small rectangles which are arranged in  $R$  rows and  $Q$  columns to form a larger rectangle. In the following discussion we shall assume, for the sake of simplicity, that  $R$  is never equal to  $Q$ .

The set of all subsets of a lattice may be partitioned by the equivalence relation of congruence. A *structure*  $\Sigma$  is taken to be any one of these disjoint equivalence classes. All elements of a structure have the same cardinality, which will be denoted by  $n_\Sigma$ . As an example, an  $r \times q$  rectangular structure  $\Sigma$  on an  $R \times Q$  rectangular array is that structure whose elements form rectangles with  $r$  rows and  $q$  columns or with  $q$  rows and  $r$  columns. Miyazaki has shown that in this case the cardinality of  $\Sigma$ , denoted by  $\nu(\Sigma)$ , is given by

$$\nu(\Sigma) = \begin{cases} (R-r+1)(Q-q+1) + (R-q+1)(Q-r+1) & \text{if } r \neq q \\ (R-r+1)(Q-r+1) & \text{if } r = q \end{cases} \quad (2.1)$$

Suppose that  $m$  particles have been distributed on the lattice  $\Lambda$ . The structure  $\Sigma$  is said to occur with occupancy  $\alpha$  in this distribution of particles if  $\alpha$  of the  $m$  particles are distributed on the sites belonging to any one element of  $\Sigma$ . For example, on an  $R \times Q$  rectangular array a nearest-neighbor pair occurs whenever a  $1 \times 2$  rectangular structure occurs with occupancy  $\alpha = 2$ .

The set of *configurations* of two structures,  $\Sigma_1$  and  $\Sigma_2$ , is the set  $U_{\Sigma_1, \Sigma_2}$  defined by

$$U_{\Sigma_1, \Sigma_2} = \{\tau = \sigma_1 \cup \sigma_2 : \sigma_1 \in \Sigma_1 \text{ and } \sigma_2 \in \Sigma_2\}$$

The set of configurations of two structures need not itself be a structure on the lattice  $\Lambda$ ; however,  $U_{\Sigma_1, \Sigma_2}$  may be partitioned into subsets of distinct cardinalities. In particular, let  $\Gamma$  denote the set of those configurations having cardinality  $n_{\Sigma_1} + n_{\Sigma_2}$ , and let  $\Gamma'$  be the complement of  $\Gamma$  in  $U_{\Sigma_1, \Sigma_2}$ . The elements of  $\Gamma$  are called *nonoverlapping*, while those of  $\Gamma'$  are said to be *overlapping*. In general, we will say that subsets  $\sigma_1$  in  $\Sigma_1$  and  $\sigma_2$  in  $\Sigma_2$  are nonoverlapping if their union  $\sigma_1 \cup \sigma_2$  lies in  $\Gamma$  and are overlapping if their union lies in  $\Gamma'$ . Note that if  $n_\tau$  denotes the cardinality of an arbitrary element  $\tau$  in  $U_{\Sigma_1, \Sigma_2}$  then  $n_\tau = n_{\Sigma_1} + n_{\Sigma_2}$  for  $\tau$  in  $\Gamma$ ; otherwise,  $n_\tau$  is strictly less than the sum  $n_{\Sigma_1} + n_{\Sigma_2}$ . Note also that the cardinality of  $\Gamma'$ , which we shall denote by  $\nu(\Gamma')$ , must be less than  $Nn_{\Sigma_1}n_{\Sigma_2}$ .

Two structures,  $\Sigma_1$  and  $\Sigma_2$ , are said to *occur simultaneously with occupancies*  $\alpha_1$  and  $\alpha_2$ , respectively, in a distribution of  $m$  particles on the

lattice if there is a configuration  $\tau = \sigma_1 \cup \sigma_2$  such that  $\alpha_1$  of the sites of  $\sigma_1$  are occupied and  $\alpha_2$  of the sites of  $\sigma_2$  are occupied. In this case the two structures are said to occur simultaneously in the configuration  $\tau$ . For the remaining part of this paper the phrase “with occupancies  $\alpha_1$  and  $\alpha_2$ ” will be omitted, as in this last definition, whenever the condition is clearly implied by the context. Let the number of sites of the configuration  $\tau$  that are occupied in the distribution be denoted by  $\alpha_\tau$ . If  $\tau$  is an element of  $\Gamma$ , then  $\alpha_\tau = \alpha_1 + \alpha_2$ ; otherwise,  $\alpha_\tau$  may be either less than or equal to the sum  $\alpha_1 + \alpha_2$ .

The extension of the above definitions to the set of configurations of  $l$  structures,  $\Sigma_1, \dots, \Sigma_l$ , and to the simultaneous occurrence of structures  $\Sigma_1, \dots, \Sigma_l$  with occupancies  $\alpha_1, \dots, \alpha_l$  is straightforward.

The *configurational ensemble*  $\mathfrak{S}_m(\Lambda)$  for the distribution of  $m$  particles on a lattice  $\Lambda$  of cardinality  $N$  is a set of duplicates of  $\Lambda$ , each with a different distribution of the  $m$  particles among the  $N$  sites. The cardinality of  $\mathfrak{S}_m(\Lambda)$  is  $\binom{N}{m}$ . We may consequently consider  $\mathfrak{S}_m(\Lambda)$  as a sample space whose points are each assigned the equal *a priori* probability  $\left(\binom{N}{m}\right)^{-1}$ .

For each element of  $\mathfrak{S}_m(\Lambda)$ , the expected number of particles at any site is  $m/N$ . This result may be calculated as an ensemble average per site in the following way. The number of times a fixed site occurs occupied in the ensemble is the number of arrangements of the remaining  $m-1$  particles among the remaining  $N-1$  sites. Since there are  $N$  single sites on the lattice, the ensemble average per site is given by

$$p = \frac{\sum_{\lambda \in \Lambda} \binom{N-1}{m-1}}{N \binom{N}{m}} = \frac{\binom{N-1}{m-1}}{\binom{N}{m}} = \frac{m}{N} \quad (2.2)$$

The ensemble average (2.2) may be generalized to the ensemble expectation of the number of simultaneous occurrences of  $l$  structures  $\Sigma_1, \dots, \Sigma_l$  with occupancies  $\alpha_1, \dots, \alpha_l$ , respectively. The generalization is expedited by the introduction of certain random variables. The variable  $X_{\Sigma_1, \dots, \Sigma_l}^\tau$  is taken to be that random variable which assumes the value 1 on those elements of the ensemble for which  $\Sigma_1, \dots, \Sigma_l$  occur simultaneously in the configuration  $\tau$  and the value zero otherwise. The total number of simultaneous occurrences of  $\Sigma_1, \dots, \Sigma_l$  is then given by the random variable

$$X_{\Sigma_1, \dots, \Sigma_l} = \sum_{\tau} X_{\Sigma_1, \dots, \Sigma_l}^\tau$$

where the summation ranges over the set  $U_{\Sigma_1, \dots, \Sigma_l}$  of all configurations.

We now consider the total number of simultaneous occurrences throughout the entire ensemble of structures  $\Sigma_1, \dots, \Sigma_l$  in the configuration  $\tau$ . If  $\tau$  is a nonoverlapping configuration, then  $\alpha_\tau$  is well defined:  $\alpha_\tau = \alpha_1 + \dots + \alpha_l$ . Moreover, if  $\tau = \sigma_1 \cup \sigma_2 \cup \dots \cup \sigma_l$ , then exactly  $\alpha_1$  of the sites of  $\sigma_1$  must be occupied, exactly  $\alpha_2$  of the sites of  $\sigma_2$  must be occupied, and so on. The number  $C_\tau$  of ways of arranging  $\alpha_\tau$  of the  $m$  particles in  $\tau$  and  $m - \alpha_\tau$  of the particles on the remaining sites of  $\Lambda$  is therefore

$$C_\tau = \binom{N - n_\tau}{m - \alpha_\tau} \prod_{k=1}^l \binom{n_{\Sigma_k}}{\alpha_k}, \quad \tau \in \Gamma$$

Note that  $C_\tau$  is the same for all configurations  $\tau$  in  $\Gamma$ . We will denote this value by  $C_\Gamma$ . If  $\tau$  is an element of  $\Gamma'$ , on the other hand,  $\alpha_\tau$  may take on a range of values so that  $C_\tau$  may be written as a sum of terms each less than or equal to  $C_\Gamma$ . Since there can be no more than  $2^{n_{\Sigma_1} + n_{\Sigma_2} + \dots + n_{\Sigma_l} - n_\tau}$  such terms, we therefore obtain

$$C_\tau \leq 2^{n_{\Sigma_1} + n_{\Sigma_2} + \dots + n_{\Sigma_l} - n_\tau} C_\Gamma, \quad \tau \in \Gamma'$$

The expected number of simultaneous occurrences of  $\Sigma_1, \dots, \Sigma_l$  is given by

$$E(X_{\Sigma_1, \dots, \Sigma_l}) = \sum_{\tau} \binom{N}{m}^{-1} C_\tau$$

where the summation ranges over the set of all configurations. When  $\tau$  is an element of  $\Gamma$ , each term  $C_\Gamma \binom{N}{m}^{-1}$  is an element of the multihypergeometric distribution:

$$C_\Gamma \binom{N}{m}^{-1} = \frac{\binom{n_\tau}{\alpha_\tau} \binom{N - n_\tau}{m - \alpha_\tau}}{\binom{N}{m}} \prod_{k=2}^l \frac{\binom{n_{\Sigma_1} + \dots + n_{\Sigma_{k-1}}}{\alpha_1 + \dots + \alpha_{k-1}} \binom{n_{\Sigma_k}}{\alpha_k}}{\binom{n_{\Sigma_1} + \dots + n_{\Sigma_k}}{\alpha_1 + \dots + \alpha_k}} \quad (2.3)$$

The mean  $\mu_{\Sigma_1, \dots, \Sigma_l}$  of the random variable  $Y_{\Sigma_1, \dots, \Sigma_l} = N^{-l} X_{\Sigma_1, \dots, \Sigma_l}$  is the density of simultaneous occurrences of  $\Sigma_1, \dots, \Sigma_l$  per  $l$ -tuple of lattice sites, and is therefore the ensemble expectation which generalizes (2.2):

$$\begin{aligned} \mu_{\Sigma_1, \dots, \Sigma_l} &= N^{-l} E(X_{\Sigma_1, \dots, \Sigma_l}) \\ &= \sum_{\tau} N^{-l} \binom{N}{m}^{-1} C_\tau \end{aligned}$$

The task now at hand is the evaluation of the limit of  $\mu_{\Sigma_1, \dots, \Sigma_l}$  as  $m$  and  $N$  each becomes large in such a way that the coverage  $\theta = m/N$  remains constant. This limit will be denoted by a plain limit symbol:

$$\mu_{\Sigma_1, \dots, \Sigma_l}(\theta) = \lim \mu_{\Sigma_1, \dots, \Sigma_l}$$

**2.2. Computation of Ensemble Expectations.** We first consider the case  $l=2$  and  $\Sigma_1 \neq \Sigma_2$ . Since the set  $\{\Gamma, \Gamma'\}$  forms a partition of  $U_{\Sigma_1, \Sigma_2}$ , we have

$$\mu_{\Sigma_1, \Sigma_2} = \sum_{\tau \in \Gamma} C_{\tau} \binom{N}{m}^{-1} + \sum_{\tau \in \Gamma'} C_{\tau} \binom{N}{m}^{-1}$$

The second term may be estimated by recalling that each element of the multihypergeometric distribution has magnitude less than unity, so that

$$\begin{aligned} \lim \left[ N^{-2} \sum_{(\tau \in \Gamma')} C_{\tau} \binom{N}{m}^{-1} \right] &\leq \lim \left[ N^{-2} \sum_{(\tau \in \Gamma')} 2^{n_{\Sigma_1} + n_{\Sigma_2} - n_{\tau}} \right] \\ &\leq 2^{n_{\Sigma_1} + n_{\Sigma_2}} \lim \left[ N^{-2} \nu(\Gamma') \right] \\ &\leq 2^{n_{\Sigma_1} + n_{\Sigma_2}} \lim \left[ N^{-1} n_{\Sigma_1} n_{\Sigma_2} \right] \\ &= 0 \end{aligned}$$

Thus

$$\mu_{\Sigma_1, \Sigma_2}(\theta) = \lim \left[ N^{-2} \sum_{(\tau \in \Gamma)} C_{\tau} \binom{N}{m}^{-1} \right]$$

For  $\tau \in \Gamma$ ,  $n_{\tau} = n_{\Sigma_1} + n_{\Sigma_2}$  and  $\alpha_{\tau} = \alpha_1 + \alpha_2$ ; therefore

$$\mu_{\Sigma_1, \Sigma_2}(\theta) = \lim \left[ N^{-2} \binom{N}{m}^{-1} \binom{n_{\Sigma_1}}{\alpha_1} \binom{n_{\Sigma_2}}{\alpha_2} \binom{N - n_{\Sigma_1} - n_{\Sigma_2}}{m - \alpha_1 - \alpha_2} \nu(\Gamma) \right]$$

where  $\nu(\Gamma)$  is the cardinality of  $\Gamma$ . On the other hand

$$\lim \left[ N^{-2} \binom{N}{m}^{-1} \binom{n_{\Sigma_1}}{\alpha_1} \binom{n_{\Sigma_2}}{\alpha_2} \binom{N - n_{\Sigma_1} - n_{\Sigma_2}}{m - \alpha_1 - \alpha_2} \nu(\Gamma') \right] = 0$$

Let the cardinality of the set  $U_{\Sigma_1, \Sigma_2}$  of configurations be denoted by

$\nu(U_{\Sigma_1, \Sigma_2})$ . Then since cardinality is an additive set function on finite sets,

$$\begin{aligned} \mu_{\Sigma_1, \Sigma_2}(\theta) &= \lim \left[ N^{-2} \binom{N}{m}^{-1} \binom{n_{\Sigma_1}}{\alpha_1} \binom{n_{\Sigma_2}}{\alpha_2} \binom{N - n_{\Sigma_1} - n_{\Sigma_2}}{m - \alpha_1 - \alpha_2} \nu(U_{\Sigma_1, \Sigma_2}) \right] \\ &= \binom{n_{\Sigma_1}}{\alpha_1} \binom{n_{\Sigma_2}}{\alpha_2} \theta^{\alpha_1 + \alpha_2} (1 - \theta)^{n_{\Sigma_1} + n_{\Sigma_2} - \alpha_1 - \alpha_2} \lim \left[ \frac{\nu(U_{\Sigma_1, \Sigma_2})}{N^2} \right] \end{aligned} \quad (2.4)$$

When  $\Lambda$  is an array and  $\Sigma_1$  and  $\Sigma_2$  are structures on  $\Lambda$ , the evaluation of the limit in (2.4) is made possible by the following results.

*Theorem 1.* If  $\Sigma_1 \neq \Sigma_2$ , then  $\lim[N^{-2}\nu(U_{\Sigma_1, \Sigma_2})] = \lim[N^{-2}\nu(\Sigma_1 \times \Sigma_2)]$ .

*Proof.* We first introduce some notation. Recall that  $\Gamma$  is the set of nonoverlapping elements of  $U_{\Sigma_1, \Sigma_2}$  and  $\Gamma'$  is the complement of  $\Gamma$  in  $U_{\Sigma_1, \Sigma_2}$ . Define  $\Gamma_x$  to be that set of ordered pairs  $(\sigma_1, \sigma_2)$  with  $\Sigma_1$  in  $\sigma_1$  and  $\sigma_2$  in  $\Sigma_2$ , such that  $\sigma_1 \cup \sigma_2$  is an element of  $\Gamma$ . Let  $\Gamma'_x$  be the complement of  $\Gamma_x$  in  $\Sigma_1 \times \Sigma_2$ .

Since  $\Lambda$  is an array, the perimeter of any subset of  $\Lambda$  is well defined; moreover, since each structure is a congruence class, each element of the structure has the same perimeter, which we shall denote by  $s_{\Sigma}$ . Let  $\Omega$  be that subset of  $\Gamma$  whose elements have perimeters less than  $s_{\Sigma_1} + s_{\Sigma_2}$ .  $\Omega$  is called the set of *contiguous* elements of  $U_{\Sigma_1, \Sigma_2}$ . As above let  $\Omega_x$  be that set of ordered pairs  $(\sigma_1, \sigma_2)$  in  $\Gamma_x$  such that  $\sigma_1 \cup \sigma_2$  is an element of  $\Omega$ . Subsets  $\sigma_1$  in  $\Sigma_1$  and  $\Sigma_2$  are also called contiguous if their union  $\sigma_1 \cup \sigma_2$  lies in  $\Omega$ . It follows that the correspondence from  $(\Sigma_1 \times \Sigma_2) \setminus (\Gamma'_x \cup \Omega_x)$  onto  $\Gamma \setminus \Omega$  defined by  $(\sigma_1, \sigma_2) \mapsto \sigma_1 \cup \sigma_2$ , is onto and one-to-one.

The existence of a bijection between  $(\Sigma_1 \times \Sigma_2) \setminus (\Gamma'_x \cup \Omega_x)$  and  $\Gamma \setminus \Omega$  implies that the cardinalities of the two sets are the same:

$$\nu[(\Sigma_1 \times \Sigma_2) \setminus (\Gamma'_x \cup \Omega_x)] = (\Gamma \setminus \Omega)$$

Therefore

$$\begin{aligned} \nu(\Sigma_1 \times \Sigma_2) - \nu(\Gamma) &= \nu(\Omega_x) + \nu(\Gamma'_x) - \nu(\Omega) \\ &\leq \nu(\Omega_x) + \nu(\Gamma'_x) \end{aligned}$$

The cardinalities of  $\Omega_x$  and  $\Gamma'_x$  have the upper bounds:

$$\begin{aligned} \nu(\Omega_x) &\leq \max[s_{\Sigma_1} n_{\Sigma_1} \nu(\Sigma_1), s_{\Sigma_2} n_{\Sigma_2} \nu(\Sigma_2)] \\ \nu(\Gamma'_x) &\leq \max[n_{\Sigma_1} n_{\Sigma_2} \nu(\Sigma_1), n_{\Sigma_1} n_{\Sigma_2} \nu(\Sigma_2)] \end{aligned}$$

It now follows that

$$\lim [N^{-2}\nu(\Sigma_1 \times \Sigma_2) - N^{-2}\nu(\Gamma)] = 0$$

Equivalently we may write

$$\lim [N^{-2}\nu(\Sigma_1 \times \Sigma_2)] = \lim [N^{-2}\nu(\Gamma)] = \lim [N^{-2}\nu(U_{\Sigma_1, \Sigma_2})]$$

Now the cardinality of the Cartesian product of finite sets is the product of their respective cardinalities. Thus

$$\mu_{\Sigma_1, \Sigma_2}(\theta) = \binom{n_{\Sigma_1}}{\alpha_1} \binom{n_{\Sigma_2}}{\alpha_2} \theta^{\alpha_1 + \alpha_2} (1 - \theta)^{n_{\Sigma_1} + n_{\Sigma_2} - \alpha_1 - \alpha_2} \lim \left[ \frac{\nu(\Sigma_1)}{N} \right] \lim \left[ \frac{\nu(\Sigma_2)}{N} \right]$$

When  $\Lambda$  is an  $R \times Q$  rectangular array with  $\Sigma_1$  an  $r_1 \times q_1$  ( $r_1 \neq q_1$ ) rectangular structure and  $\Sigma_2$  an  $r_2 \times q_2$  ( $r_2 \neq q_2$ ) rectangular structure, application of (2.1) yields that, as  $R$  and  $Q$  both become large and as the ratio  $m/RQ = \theta$  remains constant,

$$\mu_{\Sigma_1, \Sigma_2}(\theta) = 4 \binom{r_1 q_1}{\alpha_1} \binom{r_2 q_2}{\alpha_2} \theta^{\alpha_1 + \alpha_2} (1 - \theta)^{r_1 q_1 + r_2 q_2 - \alpha_1 - \alpha_2}$$

Note that here the two-point average depends only on the element cardinalities and occupancies of the structures involved.

The general formula for  $\mu_{\Sigma_1, \dots, \Sigma_l}(\theta)$  may be determined by following a similar line of reasoning to obtain the smoothed  $l$ -point average for structures  $\Sigma_1, \dots, \Sigma_l$  occurring simultaneously with occupancies  $\alpha_1, \dots, \alpha_l$ , respectively:

$$\begin{aligned} \mu_{\Sigma_1, \dots, \Sigma_l}(\theta) &= \binom{n_{\Sigma_1}}{\alpha_1} \dots \binom{n_{\Sigma_l}}{\alpha_l} \theta^{\alpha_1 + \dots + \alpha_l} \\ &\times (1 - \theta)^{(n_{\Sigma_1} - \alpha_1) + \dots + (n_{\Sigma_l} - \alpha_l)} \lim \left[ \frac{\nu(\Sigma_1)}{N} \right] \dots \lim \left[ \frac{\nu(\Sigma_l)}{N} \right] \end{aligned} \tag{2.5}$$

In the case of a rectangular lattice with rectangular structures  $\Sigma_1, \dots, \Sigma_l$  of dimensions  $r_1 \times q_1, \dots, r_l \times q_l$ , respectively, we have

$$\begin{aligned} \mu_{\Sigma_1, \dots, \Sigma_l}(\theta) &= 2^l \binom{r_1 q_1}{\alpha_1} \dots \binom{r_l q_l}{\alpha_l} \theta^{\alpha_1 + \dots + \alpha_l} \\ &\times (1 - \theta)^{(r_1 q_1 - \alpha_1) + \dots + (r_l q_l - \alpha_l)} \end{aligned} \tag{2.6}$$

where  $r_i \neq q_i$  for  $i = 1, 2, \dots, l$ . Again the limit has been taken as both  $R$  and  $Q$  become large.

*Theorem 2.* If  $\Sigma_1 = \Sigma_2$ , then  $\lim[N^{-2\nu}(U_{\Sigma_1, \Sigma_1})] = \frac{1}{2} \lim[N^{-2\nu}(\Sigma_1 \times \Sigma_1)]$ .

*Proof.* Again consider the correspondence  $(\sigma_1, \sigma_2) \rightarrow \sigma_1 \cup \sigma_2$  for  $(\sigma_1, \sigma_2)$  in  $(\Sigma_1 \times \Sigma_1) \setminus (\Gamma'_x \cup \Omega_x)$ . If  $(\sigma_1, \sigma_2)$  and  $(\sigma'_1, \sigma'_2)$  are both in  $(\Sigma_1 \times \Sigma_2) \setminus (\Gamma'_x \cup \Omega_x)$ , and if  $\sigma_1 \cup \sigma_2 = \sigma'_1 \cup \sigma'_2$ , then either  $(\sigma_1, \sigma_2) = (\sigma'_1, \sigma'_2)$  or  $(\sigma_1, \sigma_2) = (\sigma'_2, \sigma'_1)$ . The correspondence is therefore two-for-one on  $(\Sigma_1 \times \Sigma_1) \setminus (\Gamma'_x \cup \Omega_x)$  and the result follows as in the proof of Theorem 1.

The ensemble average per site for the occurrence of a structure  $\Sigma$  twice simultaneously, once with occupancy  $\alpha_1$  and once with occupancy  $\alpha_2$ , is therefore

$$\mu_{\Sigma, \Sigma}(\theta) = \frac{1}{2} \binom{n_{\Sigma}}{\alpha_1} \binom{n_{\Sigma}}{\alpha_2} \theta^{\alpha_1 + \alpha_2} (1 - \theta)^{2n_{\Sigma} - \alpha_1 - \alpha_2} \left\{ \lim \left[ \frac{\nu(\Sigma)}{N} \right] \right\}^2 \quad (2.7)$$

When  $\Lambda$  is a rectangular array and  $\Sigma$  an  $r \times q$  ( $r \neq q$ ) rectangular structure on  $\Lambda$ , the limiting average is

$$\mu_{\Sigma, \Sigma}(\theta) = 2 \binom{rq}{\alpha_1} \binom{rq}{\alpha_2} \theta^{\alpha_1 + \alpha_2} (1 - \theta)^{2rq - \alpha_1 - \alpha_2}$$

In particular, for the simultaneous occurrence of two-nearest neighbor pairs ( $n_{\Sigma} = 2$ ,  $\alpha_1 = \alpha_2 = 2$ ):

$$\mu_{\Sigma, \Sigma}(\theta) = 2\theta^4$$

Let  $\sigma_1, \dots, \sigma_l$  be  $l$  nonoverlapping, noncontiguous elements of  $\Sigma$ . Under the correspondence  $(\sigma_1, \dots, \sigma_l) \mapsto \sigma_1 \cup \dots \cup \sigma_l$ , there are  $l!$   $l$ -tuples which are mapped into the same image set. The correct generalization of (2.6), therefore, to  $l$  simultaneous occurrences of the structure  $\Sigma$  with occupancies  $\alpha_1, \dots, \alpha_l$  is

$$\begin{aligned} \mu_{\Sigma, \dots, \Sigma}(\theta) &= \frac{1}{l!} \binom{n_{\Sigma}}{\alpha_1} \dots \binom{n_{\Sigma}}{\alpha_l} \theta^{\alpha_1 + \dots + \alpha_l} \\ &\times (1 - \theta)^{ln_{\Sigma} - \alpha_1 - \dots - \alpha_l} \left\{ \lim \left[ \frac{\nu(\Sigma_l)}{N} \right] \right\}^l \end{aligned} \quad (2.8)$$

When  $\Sigma$  is an  $r \times q$  rectangular structure on a rectangular array, (2.7)



becomes

$$\mu_{\Sigma, \dots, \Sigma}(\theta) = \frac{2^l}{l!} \binom{rq}{\alpha_1} \dots \binom{rq}{\alpha_l} \theta^{\alpha_1 + \dots + \alpha_l} (1 - \theta)^{lrq - \alpha_1 - \dots - \alpha_l} \quad (2.9)$$

### 3. CONCLUSION

The limiting behavior of the  $l$ -point ensemble expectations of the number of simultaneous occurrences of  $l$  structures when indistinguishable single particles are distributed on a lattice has been calculated in (2.5) and (2.8). The expressions involve no restrictions on the lattice geometry. Averages for various structures on specific geometrical arrays, such as rectangular and hexagonal arrays, may be calculated directly from the general results.

It is also worth remarking that even though the lattice  $\Lambda$  has here been taken to be two-dimensional, the method employed in calculating the  $l$ -point expectations may be immediately generalized to lattices in higher dimensions.

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