ENTROPY OF THE MONOMER–TRIMER SYSTEM ON A HIERARCHICAL LATTICE

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The monomer–trimer model is studied on the fractal 3-simplex lattice. Configurations are enumerated by an exact system of recurrence relations. Asymptotic forms for the number of pure trimer and monomer–trimer configurations of equal weights as well as entropy are found. The asymptotic form in the close-packed limit differs from the one obtained for dimers on the square lattice. By introducing monomer fugacity, configurations are classified according to the number of monomers (or trimers), and the problem is formulated in the grand canonical ensemble. The average number of monomers and entropy are calculated as functions of fugacity. Entropy as a function of trimer fraction coverage shows qualitatively similar behavior to that found on the square lattice.

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1. Introduction

In the 1930s, Fowler and Rushbrooke [1] introduced the monomer–dimer model in order to represent a liquid mixture of differently-sized molecules. In this model, a monomer occupies one lattice site, whereas a dimer occupies two adjacent lattice sites. Double occupancy of sites is forbidden. The main question was to find the number of ways in which a lattice can be covered with a mixture of monomers and dimers. Although simple, the problem has not been solved exactly on any periodic lattice yet (except in one dimension). Over the years, the model has been extensively applied in surface physics as a model for the adsorption of diatomic molecules. Its simplified version, the so-called close-packed dimer limit, in which the lattice is completely covered by dimers, was solved analytically on planar lattices [2–5]. The problem was generalized to include rectilinear trimers [6–8], and moreover, rectilinear k-mers [9–11] in the studies on the orientational ordering of long rod-like molecules related to liquid crystals. In the k-mer model, k connected monomers singly occupy k contiguous lattice sites.

Due to the intractability of models on periodic lattices (only some specific cases are solved exactly, for example, triangular (V-shaped) trimers on the triangular lattice in the close-packed trimer limit [12]), the problems are usually posed on some graphs or lattices on which exact or asymptotic solutions can be drawn. For this purpose, fractal lattices with finite ramification have proven to be very suitable, because their hierarchical structure enables the recurrent enumeration of configurations. Moreover, the lack of translational symmetry makes them convenient for the simulation of inhomogeneous substrates in adsorption phenomena (the application of the model for adsorption on the homogeneous substrate is considered, for example, in [13]).

Although the close-packed dimer model and the monomer–dimer model have been studied on fractal lattices [14–17], the monomer–trimer model has not yet been studied in this way. In this paper, we take a step forward and study the monomer–trimer system on the fractal 3-simplex lattice. We aim at finding out what effects the fractal structure has on the behavior of the model. Trimers of all possible shapes on this lattice are considered. An exact set of recurrence equations is constructed for the enumeration of close-packed trimer configurations, from which the asymptotic growth constant (or equivalently entropy) is found. Then, by extending the recurrent technique and applying the grand canonical ensemble, the entropy of the monomer–trimer model and the density of trimers are calculated numerically as functions of monomer fugacity. Finally, the plot of entropy *versus* density is presented.

Section 2 is concerned with pure trimers, Section 3 with the mixture of monomers and trimers, whereas discussion and conclusions are presented in Section 4.

2. The close-packed trimers

In this section, the 3-simplex lattice relevant to this study is described, after which the derivation of recurrence equations for the close-packed trimers is outlined. The asymptotic expression for the number of close-packed trimer configurations and the entropy per lattice site in the thermodynamic limit are determined.

2.1. The 3-simplex lattice

The 3-simplex lattice [18, 19] is a fractal lattice embedded in two-dimensional space. It is constructed in an iterative manner, starting with a unit triangle as an initiator. In each step, the generator of the r^{th} order ($G^{(r)}$) is obtained by connecting three generators of the order of $r-1$ ($G^{(r-1)}$) by three bonds, as shown in the first three steps of construction in Fig. 1. The complete lattice is obtained when the number of steps tends to infinity. The generator of the r^{th} order comprises 3 generators of the order of $r-1$ (as sub-

generators), 3^2 generators of the order of $r-2,\ldots$ and 3^{r-1} unit triangles. It has $N_r = 3^r$ lattice sites and $N_b = 3(3^r-1)/2$ bonds. Its coordination number is three. The lattice can be obtained from a two-dimensional Sierpinski gasket by splitting the vertices of its neighboring triangles. It is equivalent to the infinite graph of the Hanoi tower, a commonly used graph in physics and combinatorial mathematics [20, 21].

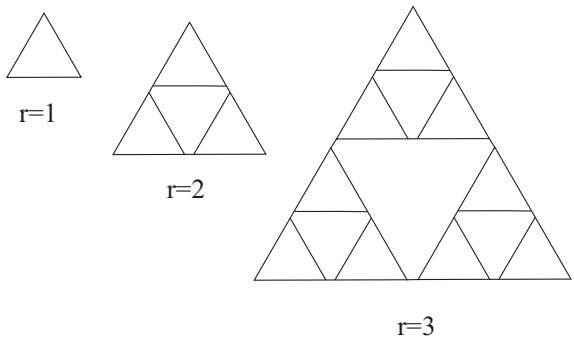

Fig. 1. The first three generators of the 3-simplex lattice. The complete lattice is obtained when $r \to \infty$.

2.2. Recurrence equations for pure trimers

A trimer can be considered as a triatomic molecule which occupies three adjacent lattice sites. In the close-packed trimer model, all lattice sites are singly occupied with units that belong to trimers (there are no single monomer units *i.e.* vacancies). We consider flexible trimers of different shapes that can exist on the 3-simplex lattice: rectilinear and bent at angles of 60 and 120 degrees. One configuration in which pure trimers cover all lattice sites of the generator $G^{(4)}$ is presented in Fig. 2. As one can observe, trimer configurations on sub-generators are such that trimers either completely belong to the same sub-generator (internal trimers) or they protrude along the bonds between neighboring sub-generators, in which case we say that they are external trimers. In Fig. 2, the encircled configuration on $G^{(2)}$ in the right corner of $G^{(4)}$ contains only internal trimers, whereas another encircled configuration contains parts of two external trimers. External trimers start at the corner vertex of one sub-generator, enter the neighboring sub-generator via its corner vertex, and end in one of its two remaining nearest neighboring vertices (starting and ending points are symmetrical). Therefore, each external trimer occupies one or two lattice sites on a sub-generator. At most three external trimers can be associated with each sub-generator. Since each $G^{(r)}$ contains $N_r = 3^r$ vertices, due to the close packing, configurations with external trimers are permissible only if trimers altogether visit three or six vertices on the considered generator

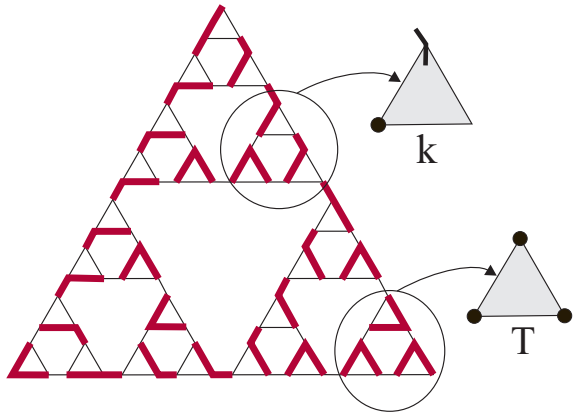

Fig. 2. Close-packed trimer covering of the fourth order generator of the 3-simplex lattice. Two possible types of configurations on the generators are encircled and shown schematically aside.

(the number of remaining vertices on the generator must be divisible by three). Some of these configurations are further forbidden due to the lattice geometry. Classifying all possible configurations on an arbitrary generator according to the occupancy of its corner vertices, we find that only two types of configurations are possible. In the configuration denoted by T, all corner vertices are occupied with internal trimers. This configuration represents all close-packed trimer configurations on the generator. In the the coarse-grained description, a generator with a T configuration is represented as a gray triangle with each corner vertex filled with a black circle representing a monomer that belongs to an internal trimer (Fig. 2). The only possible configuration with external trimers, denoted as k, is the one in which one corner vertex is occupied with a trimer from the inside, another corner vertex is occupied with the end-point of an external trimer (with a trimer from the outside), and the third corner vertex is occupied with the middle-point of another external trimer. A generator with a k configuration, as shown in Fig. 2, is depicted as a gray triangle in which one corner vertex is filled with the black circle, another is empty (the external trimer ends in this corner vertex), whereas the third corner vertex contains black line representing an external trimer which starts inside and extends out of the generator. The close-packed trimer configuration on $G^{(4)}$ shown in Fig. 2 is composed of three k configurations, one on each $G^{(3)}$.

In order to find recurrence equations for the numbers of T and k configurations, in Fig. 3, we present all possibilities to obtain a T configuration on $G^{(r+1)}$ from T and k configurations on $G^{(r)}$. Since each configuration on each of the three sub-generators $G^{(r)}$ can be combined into one configuration

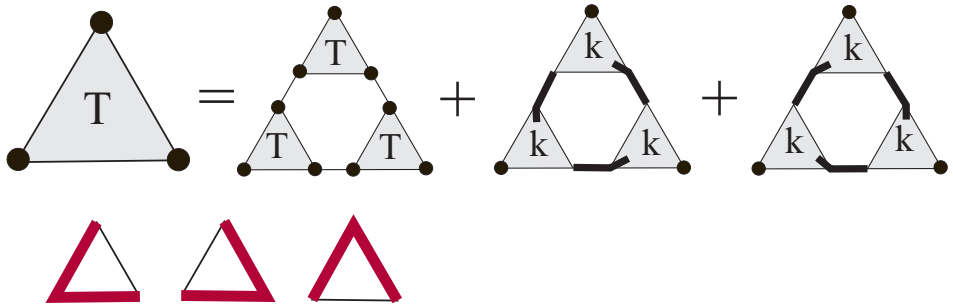

Fig. 3. Decomposition of configuration T on $G^{(r+1)}$ on its composing parts-configurations T and k on $G^{(r)}$. Initial T configurations on the unit triangle are shown in the second row.

on $G^{(r+1)}$, the number of configurations on $G^{(r+1)}$ can be obtained as the product of the number of configurations on its sub-generators. Denoting the numbers of T and k configurations on an arbitrary $G^{(r)}$ as T_r and k_r, the recurrence relation for T_r, according to Fig. 3, is given by

$$T_{r+1} = T_r^3 + 2k_r^3\,. \tag{1}$$

In Fig. 4, we present all possibilities to obtain a k configuration on $G^{(r+1)}$ from T and k configurations on $G^{(r)}$, from which the recurrence relation for the variable k follows as:

$$k_{r+1} = T_r k_r^2 + k_r^3\,. \tag{2}$$

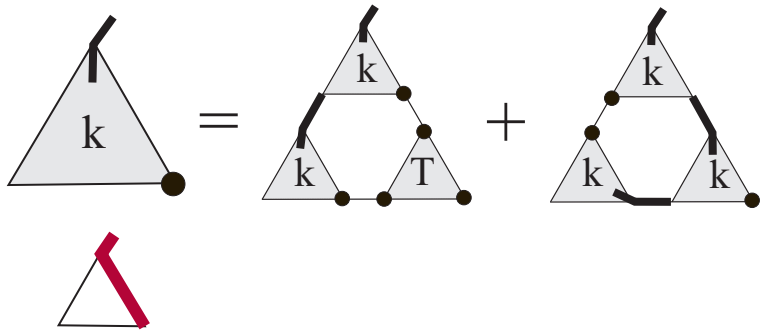

Fig. 4. Decomposition of the configuration k on $G^{(r+1)}$ on its composing parts — configurations T and k on $G^{(r)}$. The initial k configuration on the unit triangle is shown in the second row. The empty corner vertex is occupied with an external trimer from the outside.

Equations (1) and (2) form a closed system of non-linear difference equations. Initial conditions are given as $T_1 = 3$ and $k_1 = 1$, with the initial configurations illustrated in Figs. 3 and 4. Equations can be iterated and the number T_r of close-packed trimer configurations on any $G^{(r)}$ can be found explicitly. To obtain the asymptotic form, according to which the number of configurations grows with the number of lattice sites, it is convenient to introduce a new variable defined as $x_r = k_r/T_r$. Then, from (1) and (2), a new equation for variable x_r is obtained as

$$x_{r+1} = x_r^2 \frac{1 + x_r}{1 + 2x_r^3}\,, \tag{3}$$

whose fixed points x^* are obtained as solutions of the equation

$$x^* = (x^*)^2 \frac{1 + x^*}{1 + 2(x^*)^3}\,. \tag{4}$$

Among four solutions, the only real, non-negative is $x^* = 0$. It is a stable fixed point, so that iteration of equation (3) from the initial condition $x_1 = 1/3$ leads to zero. This implies that variable T_r increases much faster than k_r, and equation (1) for $r \gg 1$ takes on the asymptotic form

$$T_{r+1} \sim T_r^3\,. \tag{5}$$

The solution is $T_r \sim \omega^{3^r}$, where ω is the so-called growth constant. Expressing T_r in terms of the number of vertices $N_r = 3^r$ on $G^{(r)}$, we have

$$T_r \sim \omega^{N_r}\,. \tag{6}$$

The growth constant ω is determined from $\ln\omega = \lim_{N\to\infty} \ln T_r/N_r$. Numerical iteration gives $\ln\omega = 0.374338099718\ldots$, from which it follows that $\omega = 1.454028674046\ldots$ Since the entropy of close-packed trimer configurations on $G^{(r)}$ is given as $S_r = k_\mathrm{B} \ln T_r$, where k_B is the Boltzmann constant, the value of $\ln\omega$ represents the entropy per Boltzmann constant, per lattice site in the thermodynamic limit, *i.e.* $s = \lim_{N_r\to\infty} S_r/(k_\mathrm{B}N_r) = \ln\omega = 0.374338099718\ldots$ The entropy per trimer is three times larger.

As one can see, the asymptotic expression (6) is exponential, with no correction factor. The same form (with a different growth constant) is found for close-packed dimers on other fractal lattices [16] (close-packed dimers cannot exist on the three-simplex lattice). However, for dimers on the very large portion of the square lattice, with a free boundary (without periodic or any other boundary conditions imposed), the stretched exponential correction factor $\mu^{N^{1/2}}$ to the leading exponential is obtained [5]. More precisely,

the asymptotic expansion of the free energy consists of a leading order exponential term and a stretched exponential as a higher-order correction term. This correction is due to the 'surface' effect, *i.e.* to the smaller coordination number of $N^{1/2}$ sites on the lattice boundary. In the case of the 3-simplex lattice, all sites have the coordination number of three, except for three corner vertices of the largest generator with the coordination number of two. This negligible number of sites has no effect on the asymptotic form of dimers nor trimers.

3. The monomer–trimer system

In this section, the recurrence method for the enumeration of monomer–trimer configurations is developed. Then, the asymptotic expression for the number of configurations and the corresponding entropy are obtained. In this approach, configurations with different numbers of trimers, from zero to maximal number $N_r/3$, are all equally weighted. However, by assigning a fugacity to each monomer and applying the grand canonical ensemble, configurations with a different number of monomers (trimers) get different weights. This enables us to obtain the entropy of the monomer–trimer model as a function of density (fraction of lattice sites covered with trimers).

3.1. Recurrence equations for the monomer–trimer system

Generalization of the method of recurrence equations from Section 2 on the mixture of monomers and trimers is quite straightforward, but much more complicated. Analysis of possible types of configurations on generators shows that ten different types are possible. Similarly as in the case of pure trimers, one of them, denoted as T, represents all monomer–trimer configurations, whereas nine other types represent configurations with external trimers. In Fig. 5, one monomer–trimer configuration on $G^{(4)}$ of the 3-simplex lattice is presented together with a schematic representation of some possible types of configurations on sub-generators of the second order. In Fig. 6, all ten types of configurations are schematically represented. The black circle means that the corner vertex of a generator is occupied with a single monomer or a trimer from the inside. The black line which extends through the corner vertex represents an external trimer which starts inside the generator. A corner vertex which stays empty is occupied by an external trimer from the outside. Recurrence equations for all ten configurations are obtained from schematic representations as the one shown in Fig. 7 for the configuration T. The configuration T on $G^{(r+1)}$ can be obtained by combining different types of configurations on sub-generators $G^{(r)}$. Each type is marked inside the constituting sub-generators. This gives rise to different terms in the recurrence equation for the variable T, given by the first equation in (7). The numbers in front of triangles stand for different,

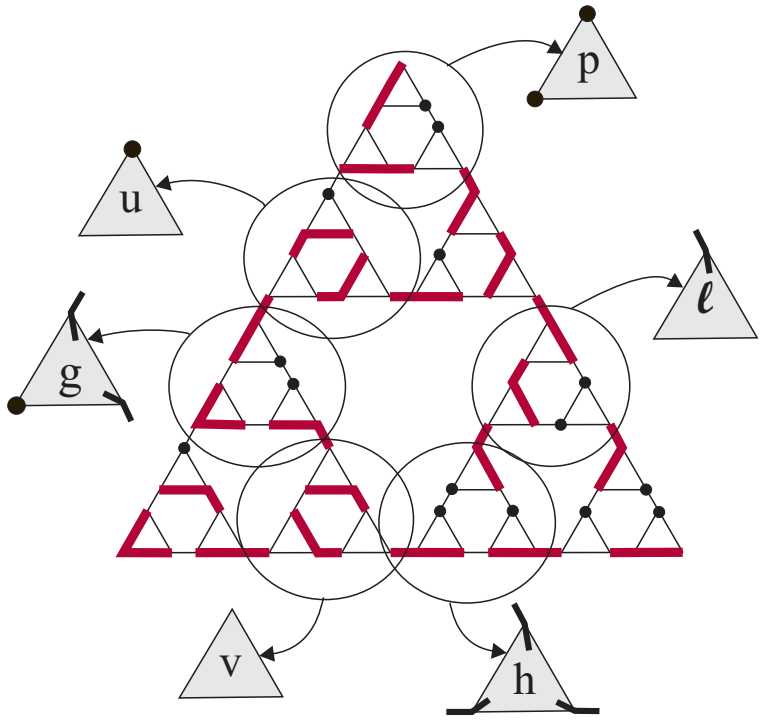

Fig. 5. Monomer–trimer configuration on the fourth order generator of the 3-simplex lattice. Some configurations on the second order generators are encircled and represented schematically aside.

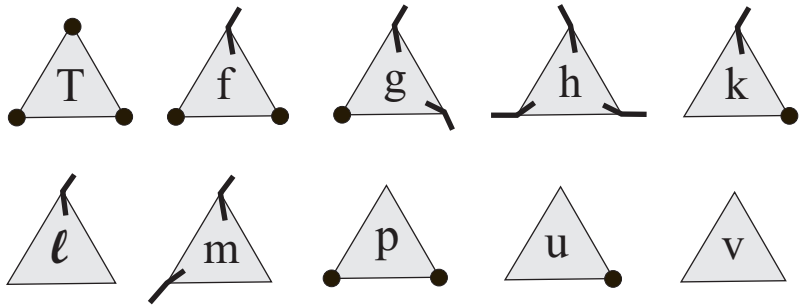

Fig. 6. Schematic representation of different types of configurations of the monomer–trimer system on generators of the 3-simplex lattice.

symmetrically-related configurations of the same type, and represent the coefficients of the terms in the recurrence equation. Recurrence equations for other configurations are obtained by similar illustrations, and altogether are given by

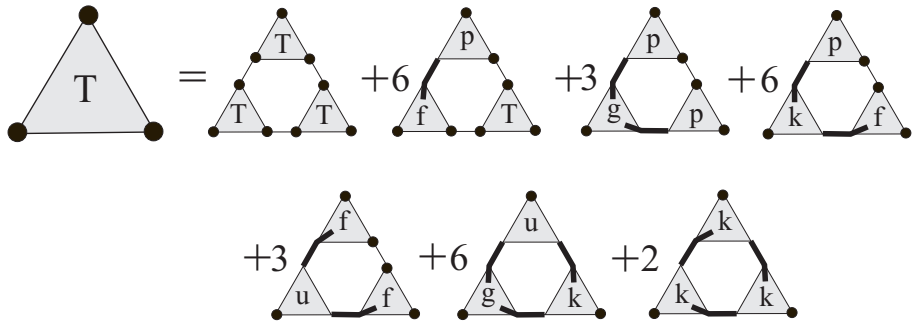

Fig. 7. Decomposition of the configuration T on $G^{(r+1)}$ on its composing parts — configurations on $G^{(r)}$.

$$
\begin{aligned}
T' &= T^3 + 6Tfp + 3gp^2 + 6fkp + 3f^2u + 6gku + 2k^3\,,\\
f' &= T^2f + 2Tfk + 2Tgp + 2f^2p + 2fk^2 + 4gkp + 2fgu + f^2l + 2fmp\\
&\quad + hp^2 + 2gkl + 2k^2m + 2gmu + 2hku\,,\\
g' &= Tf^2 + 2Tgk + 2f^2k + 2fgp + 2fkm + 2hkp + 2fgl + 2gmp + 3gk^2\\
&\quad + g^2u + 2glm + 2km^2 + 2hkl + 2hmu\,,\\
h' &= f^3 + 6fgk + 6gkm + 3hk^2 + 3g^2l + 6hlm + 2m^3\,,\\
k' &= Tfp + Tk^2 + Tgu + f^2u + 2fkp + gp^2 + 2fkl + 2kmp + fgv + glp\\
&\quad + fmu + hpu + 3gku + k^3 + gl^2 + 3klm + m^2u + gmv + hkv + hlu\,,\\
l' &= fp^2 + 2k^2p + 2gpu + 2fku + 3k^2l + 4kmu + 2gkv + 2glu + hu^2\\
&\quad + 4l^2m + 2m^2v + 2hlv\,,\\
m' &= f^2p + 2gkp + 2fk^2 + 2fgu + 3k^2m + 2hku + 4gkl + 2gmu + g^2v\\
&\quad + 4lm^2 + 2hl^2 + 2hmv\,,\\
p' &= T^2p + 2Tfu + 2Tkp + 2fp^2 + 4fku + 2gpu + 2k^2p + f^2v + 2flp\\
&\quad + mp^2 + 2gkv + 2k^2l + 2glu + 2kmu\,,\\
u' &= Tp^2 + 2Tku + 2fpu + 2kp^2 + 2flu + 2mpu + 2fkv + 2klp + gu^2\\
&\quad + 3k^2u + 2glv + 2kl^2 + 2kmv + 2lmu\,,\\
v' &= p^3 + 6kpu + 6klu + 3mu^2 + 3k^2v + 6lmv + 2l^3\,,
\end{aligned}
\tag{7}
$$

where the subscript $r+1$ is replaced with the prime symbol, whereas r is omitted, for simplicity. The sum of coefficients in each equation is twenty seven. Initial conditions are given as: $T_1 = 4$, $f_1 = 2$, $g_1 = 0$, $h_1 = 0$, $k_1 = 1$, $l_1 = 0$, $m_1 = 0$, $p_1 = 1$, $u_1 = 1$, $v_1 = 1$.

Iterating the system of equations (7) from initial values, we find that all ratios f_r/T_r, g_r/T_r, …, v_r/T_r tend to constant values when $r \to \infty$, implying that $T_{r+1} \sim \text{const.}\ T_r^3$ when $r \to \infty$. Then, it follows that $T_r \sim A\omega^{3^r}$,

where A is some constant. Therefore, the number of all monomer–trimer configurations increases with the number of lattice sites as $T_r \sim A\omega^{N_r}$. The logarithm of the growth constant ω in this case is found to be $\ln\omega = 0.597237947983\ldots$ which is also the entropy per site in the thermodynamic limit.

3.2. The grand canonical ensemble approach

In the previous consideration, calculated entropy corresponds to monomer-trimer configurations with all possible numbers of trimers. To find entropies which correspond to a fixed, average number of trimers, we assign a fugacity (activity) $x = \exp(\mu/kT)$ to each single monomer (equivalently, a fugacity can be assigned to a monomer that belongs to a trimer, but in our case, the former choice turned out to be simpler). In the previous expression, μ is the chemical potential and T is the absolute temperature. On a lattice with N_s sites, each monomer–trimer configuration consists of N monomers and $(N_s - N)/3$ trimers. The grand canonical partition function is

$$\Xi(x) = \sum_{N=0}^{N_s} x^N Z_N \,, \tag{8}$$

where the sum runs over all possible numbers of monomers (trimers). Z_N is the partition function in the canonical ensemble, which in our model is equal to the number of configurations in which N monomers and $N_t = (N_s - N)/3$ trimers can be arranged on a lattice. That is, Z_N is the 'partition function' in the microcanonical ensemble, since all configurations have equal energy taken to be zero. The only energy associated with the model is the excluded volume effect which is accounted for by single occupancy of sites. In the thermodynamic limit, the number of sites N_s tends to infinity. From the grand canonical partition function Ξ, the average number of monomers can be obtained as

$$\langle N\rangle = x\frac{\partial \ln \Xi}{\partial x} \,. \tag{9}$$

Since the internal energy is zero, the expression $U - TS - \mu\langle N\rangle = -kT\ln\Xi$ gives the entropy

$$S = k\ln\Xi - (k\ln x)\langle N\rangle \,. \tag{10}$$

The average density of monomers (the monomer fraction coverage) is given by

$$\rho_m = \lim_{N_s\to\infty} \frac{\langle N\rangle}{N_s} \,, \tag{11}$$

while the average density of monomers connected into trimers (trimer fraction coverage) is $\rho = 1 - \rho_m$ (density of trimers is $\rho_t = \rho/3$). From equations

(10) and (11), it follows that the entropy per site, in the thermodynamic limit, is

$$s = k \lim_{N_s \to \infty} \frac{\ln \Xi}{N_s} - (k \ln x)\rho_m \,. \tag{12}$$

In the limit when $x \to \infty$ *i.e.* $\mu \to \infty$, $\rho_m \to 1$ ($\rho \to 0$). In this case, the whole lattice is covered with monomers, which can be done in just one way, leading to zero entropy. In the limit when $x \to 0$ *i.e.* $\mu \to -\infty$, the close-packed trimer limit is obtained. In this limit, the density of monomers tends to zero, whereas trimer fraction coverage tends to one ($\rho \to 1$). For $x = 1$ ($\mu \to 0$ or $T \to \infty$), the model reduces to unweighted model in which $\Xi(1)$ represents the overall number of monomer–trimer configurations with all possible numbers of monomers (trimers).

The unweighted monomer–trimer model analyzed in the previous subsection can very simply be turned into a weighted model. Namely, we will now assign a weight x to each monomer in monomer–trimer configurations, which can be done by assigning weights to initial configurations. Instead of numbers of initial configurations T_1, f_1, g_1, …, v_1, we now have initial weights of the configurations given by: $T_1 = x^3 + 3$, $f_1 = 2x$, $g_1 = 0$, $h_1 = 0$, $k_1 = 1$, $l_1 = 0$, $m_1 = 0$, $p_1 = 1$, $u_1 = x$, and $v_1 = 1$. In this context, T_r becomes a polynomial in x with the maximum degree equal to N_r, which is the number of sites N_s of the r^{th} order generator. In the thermodynamic limit $N_r \to \infty$. The coefficient of the term with x^N is equal to the number of monomer–trimer configurations which consist of N monomers and $(N_s - N)/3$ trimers. Comparing this observation with expression (8), one can see that T_r becomes the grand canonical partition function, from which the average density of monomers (11) and entropy (12) can be calculated numerically for each particular value of x. However, the calculation of the average number of monomers and density requires partial derivatives of the grand canonical partition function with respect to x, so that besides ten variables already introduced, ten new variables are defined as their partial derivatives with respect to x. Recurrence equations for new variables are obtained from the system given by (7). By the simultaneous iteration of twenty recurrence equations, entropy is calculated numerically and presented in Fig. 8 (circles) as a function of density (fraction of sites covered by trimers, ρ). In the same figure, the entropy of the monomer–dimer system (squares) obtained in [17] is also presented for comparison. Some values of fugacity x with the corresponding values of density and entropy are given in Table 1. Results in the table are presented with four significant figures, although the values can be calculated with almost arbitrarily high accuracy.

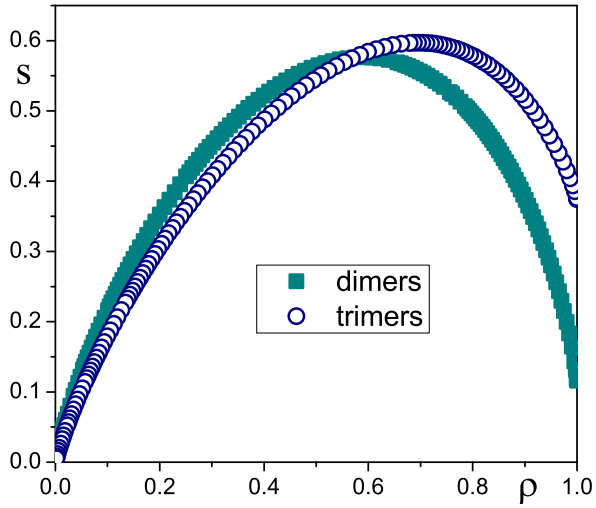

Fig. 8. Entropy of the monomer–trimer system on the 3-simplex lattice as a function of density, obtained in this paper (blue circles). Also, the entropy of the monomer–dimer model on the same lattice obtained in [17] (green squares) is presented.

Table 1. Values of density and entropy of the monomer–trimer system on the 3-simplex lattice for some chosen values of x. The last digit is rounded off.

x	0.01	0.05	0.1	0.2	0.4	0.6	0.8	0.9
ρ	0.9999	0.9994	0.9957	0.9732	0.9011	0.8297	0.7615	0.7282
s	0.3743	0.3762	0.3856	0.4277	0.5154	0.5655	0.5901	0.5955
x	1.0	1.1	1.5	2	3	5	8.0	15.0
ρ	0.6954	0.6630	0.5385	0.4012	0.2105	0.06354	0.01702	0.002653
s	0.5972	0.5957	0.5638	0.4880	0.3183	0.1248	0.04115	0.008072

4. Summary and conclusions

In this paper, the monomer–trimer model is studied on the fractal 3-simplex lattice. A simpler variant, the close-packed trimer model in which the whole lattice is covered with trimers, with no overlap or vacancies, is considered first. From the exact system of recurrence equations, it is found that the number of trimer configurations asymptotically increases as $T_r \sim \omega^{N_r}$. The growth constant ω, which determines the entropy per lattice site in the thermodynamic limit, is found numerically. The entropy is $s_t = \ln \omega = 0.374338099718\ldots$ The exponential growth, with no correction

factor, is also found for close-packed dimers on other fractal lattices [16]. The correction factor in the close-packed limit is expected on a very large subset of a lattice, which has a free boundary, due to the smaller coordination number of boundary sites. Indeed, in the close-packed dimer problem on the square lattice, the asymptotic form consists of the leading exponential factor and the stretched exponential as a perimeter correction [5]. On the fractal lattice considered here, a negligible number of sites of the largest generator have a smaller coordination number, and corrections do not appear. However, in the case of Hamiltonian walks, which can be considered as the k-mer model in the limit when $k \to \infty$, the stretched exponential factor exists on some fractal lattices [22]. It exists on the 4-simplex lattice for example, whereas for close-packed dimers on the same lattice, it does not. Then, one may wonder whether it appears in the limit when $k \to \infty$, or it appears for some finite k, in which case one would like to know this marginal k-value. A generalization of the trimer to the k-mer problem for an arbitrary $k > 3$ might not be so straightforward on fractal lattices, and is left for some future research. The origin of the stretched exponential factor for Hamiltonian walks on fractal lattices is a subtle effect of corner vertices, discussed in [23, 24].

The method of recurrence equations from Section 2 is extended to the monomer–trimer unweighted problem, which turned out to be much more complicated than the trimers themselves. Ten variables and recurrence equations were necessary to enumerate all monomer–trimer configurations with an arbitrary number of trimers. In this case the entropy is found to be $s = \ln \omega = 0.597237947983\ldots$, larger than expected, since it includes all possible numbers of trimers.

In order to find the entropy as a function of the average density of monomers connected into trimers ρ, a fugacity which controls the number of monomers (trimers) in the system is introduced and the grand canonical ensemble is applied. Entropy is calculated numerically and presented in Fig. 8 as a function of ρ. When $x \to 0$, $\rho \to 0$, and entropy tends to zero, the lattice is completely covered with monomers. When $x \to \infty$, $\rho \to 1$, the close-packed trimer limit is reached. In this limit, the whole lattice is covered with sole trimers and entropy reduces to s_t. Finally, for $x = 1$, the model reduces to an unweighted model. This corresponds to the maximum value of entropy $s = 0.597237947983\ldots$ for the density $\rho = 0.695376612042\ldots$ Entropies of the monomer–trimer (studied here) and the monomer–dimer system [17] on the 3-simplex lattice are compared in Fig. 8. One can see that there are slight differences between entropies of two models at low densities, and that they increase with the density and become significant at close packing. The maximum entropy of monomer–trimers (with all shapes of trimers) is higher than the maximum entropy of monomer–dimers ($s_{\mathrm{md}} = 0.57646430\ldots$ [17]).

It is also achieved at a higher density than for monomer–dimers. This effect is also observed on the square lattice [10], where it is shown that in the general case of k-mers, the density at which the maximum entropy occurs increases with k. However, it is found that the maximum entropy of the k-mer system on the square lattice is a non-monotonic function of k, exhibiting the maximum value for $k = 4$ [10]. It would be interesting to find out whether similar behavior occurs on fractal lattices. Also, the k-mer model with $k = 2$ and $k = 3$ with the addition of various energy weights (as in [8, 25]) would be worthwhile to study, since its critical behavior on fractal lattices might be absent or different from the one found on periodic lattices [17, 26, 27].

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