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# ENUMERATION OF DIMER CONFIGURATIONS ON A FRACTAL LATTICE

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**Abstract:** In this paper, we present a solution to the close-packed dimer problem on a fractal lattice. The dimer model is canonical model in statistical physics related with many physical phenomena. Originally, it was introduced as a model for adsorption of diatomic molecules on surfaces. Here we assume that the two dimensional substrate on which the adsorption occurs is nonhomogeneous and we represent it by the modified rectangular (MR) fractal lattice. Self-similarity of the fractal lattice enables exact recursive enumeration of all close-packed dimer configurations at every stage of fractal construction. Asymptotic form for the overall number of dimer coverings is determined and entropy per dimer in the thermodynamic limit is obtained.

**Keywords:** dimer configurations, adsorption, fractals, entropy.

## 1. INTRODUCTION

Studying liquid mixtures of unequally sized molecules Fowler and Rushbrooke [1] in 1937 introduced a lattice model for molecular configurations. In this monomer-dimer model, smaller molecules (i.e. monoatomic molecules) are allowed to occupy one lattice point and are called monomers, while bigger molecules (i.e. diatomic molecules) occupy two adjacent lattice points and are called dimers. Each lattice site is occupied by either a monomer or dimer molecule, and monomer-dimer problem in its simplest form can be stated as the problem of enumeration of all distinct configurations that can exist on a lattice of a given geometry. It is a hard combinatorial problem that has not been solved exactly yet on two- or three-dimensional lattices, but with some reductions in the model, exact solutions are possible. If the number of monomers is reduced to zero, and the whole lattice is covered with dimers, fully-packed or close-packed dimer model is obtained. It has generally been shown that the problem of close-packed dimers or perfect matchings, as it is called in graph theory, can be solved exactly for planar lattices [2], and, specifically, the number of close-packed dimers on rectangular (square) lattice has been determined in [2,3], and independently in [4,5,6]. Importance of close-packed dimer model in theoretical physics has emerged when one of the most elegant solutions for the two-dimensional Ising model has been established from the equivalence of the Ising model and close-packed dimer model on the same planar graph [7]. Among connections with other systems and models in physics and mathematics, we mention just a few: Coulomb gas, conformal field theory and associated height models [8, 9], topological string A-model [10], spanning trees [11,12] and domino tillings[13].

Besides the rectangular lattice, close-packed dimer model has been studied on other translationary invariant lattices and graphs with different boundary conditions [14−16]. On fractal lattices, one variant of dimer model has been considered in [17] and close-packed dimer model with vacancies in [18]. Fractal lattices are scale invariant and are usually considered as the intermediate lattices between translationary invariant ones and random graphs. They can often serve as a representation of some nonhomogeneous substrate on which the adsorption occurs. In the past decade, the problem of molecular adsorption on surfaces has been reinvigorated because of its technological applications such as hydrogen storage in carbon-based substrates.

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In this article, we study close-packed dimer problem on the modified rectangular (MR) fractal lattice embedded in two dimensional space. We assume that all dimer configurations have the same energy and determine the asymptotic form for the overall number of dimer configurations and the corresponding microcanonical entropy.

## 2. RECURSIVE ENUMERATION OF DIMER COVERINGS ON A FRACTAL LATTICE

In this section, we give a short introduction to fractals generally, and present an iterative construction of MR fractal lattice that is relevant for this paper. After that, we introduce a close-packed dimer model and develop a recursive method for the enumeration of all close-packed dimer configurations on MR lattice.

### 2.1. Fractals and MR fractal lattice

Most of the objects or patterns found in nature such as reliefs, coastlines, clouds, lightning, ferns, human brain, etc., are so irregular and fragmented that they cannot be described in terms of Euclidean geometry. This was first recognized by B. Mandelbrot, who in 1975 designated them as fractals, and in his book 'The fractal geometry of nature' [19], gave a unique description of such objects, as well as strange sets and curves that had been studied in mathematics (Cantor set, Koch curve, Sierpinski gasket and carpet, Menger sponge, ….) . Mandelbrot introduced criteria according to which an object can be classified as a fractal: (i) it should be sufficiently irregular and jagged, (ii) it should have many details on all length scales, (iii) its Hausdorff dimension should exceed its topological dimension. Since fractals have fine structure and details at all length scales, they are scale invariant. This means that if we take one small part of a fractal and uniformly enlarge it to the size of the whole object, they will match. This property is also called self-similarity. A small part is similar to the whole. Fractals in nature are self-similar only in average so that they are statistical fractals, while fractals in mathematics constructed by an iterative procedure are strictly self-similar, and are usually referred to as deterministic fractals. In construction of fractals in mathematics, it is customary to begin with an object of finite size and iteratively replace its parts with smaller, rescaled copies of the original, until the object of finite size with infinitely small details is reached. Another way, usually adopted in construction of fractal lattices in physics, is to start from an object of finite size and iteratively replicate it in a larger structure until infinitely large object with finite details is obtained.

Because of their outstanding properties, fractals have found diverse technological applications (some of them are fractal-shaped antennae, fractal transistors, solar panels). They are also applied in simulations and analysis of various physical phenomena especially in material sciences [20−22], in the theoretical modeling of nonhomogeneous media [23], and in the theoretical studies of the influence of the dimensionality on the nature of phase transitions [24,25].

In the present paper, we consider modified rectangular (MR) fractal lattice as a model of nonhomogeneous substrate for adsorption of diatomic molecules. Modified rectangular lattice is a deterministic fractal lattice [24] constructed in self-similar iterative manner whose first four steps are depicted in Figure 1. The first step of construction is a graph of four points in the form of a unit square. In the second step, two unit squares are joined into rectangle, while in the third step two copies of the previous rectangle are joined into the square. In each next step, two copies of the structure obtained in the previous step are joined into a rectangular or square shape, and the whole lattice is obtained repeating the process ad infinitum. Rectangle or square obtained in the *r*-th step is called *r*-th order generator and denoted by $G_r$. The number of lattice points in the *r*-th order generator is $2^{r+1}$. Fractal dimension of MR lattice is integral and equal to 2.

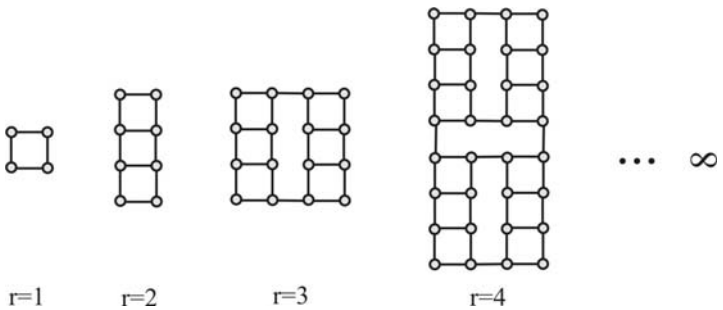


*Figure 1. Iterative construction of MR fractal lattice. The first four steps are presented, and the process should be repeated infinitely many times*

2.2. A theoretical model and a method

A dimer is a diatomic molecule, i.e. two units called monomers connected by a chemical bond. In close-packed dimer model, it is assumed that the whole lattice is covered with dimers such that no lattice site is stayed vacant. It should be stressed that only lattices with even number of lattice points can have close-packed dimer coverings, i.e. can be completely covered with dimers. If the lattice contains $N = 2M$ lattice points, then $M$ dimers can be placed on this lattice. The purpose of the present work is to determine the number of ways in which $M = 2^r$ dimers can be placed on a *r*-th order generator of MR lattice that consists of $N = 2^{r+1}$ lattice points. Self-similarity of fractal lattice enables us to construct recursive relations for the enumeration of the configurations.

In order to develop recursive enumerative scheme we refer to Figure 2, where one close-packed dimer configuration on the *5*-th order generator of MR fractal is presented. Each lattice point is occupied by a monomer bonded with adjacent monomer into a dimer. One should notice that in this hierarchically constructed $G_5$, that consists of two $G_4$, which in turn consist of two $G_3$ and so on, some of the four corner vertices of the generator of any order are occupied by the monomers paired into dimers by the monomers on the corner vertices of the neighbouring generators, while other corner monomers and 'internal' monomers form dimers by the monomers on the same generator. For the sake of simplicity, it is useful to apply the so-called coarse-graining procedure in which we overleap internal structure of the generators and associated dimer configurations, and represent real dimer configurations by the coarse-grained configurations which depict only the corner monomers. In Figure 3, coarse-graining procedure for dimer configuration given in Figure 2 is presented. Black circles represent corner monomers that form dimers with adjacent monomers on the same generator, while white circles represent corner monomers connected into dimers by the adjacent corner monomers of neighbouring generators. In the first step of course-graining procedure, internal structure of the second order generators is omitted and is shown as a shaded area, while real dimer configurations on each $G_2$ are represented only by corner monomers. In the next steps of coarse-graining procedure, dimer configurations on each $G_3$, $G_4$ and $G_5$ are represented by their coarse-grained configurations, depicting only the corner monomers of the corresponding generators. As one can see in Figure 3, for a given close-packed dimer configuration on $G_5$, there are only four possible types of coarse- grained configurations on sub-generators. This is also true for any other possible close-packed dimer configuration on the arbitrary $G_r$. These four types of coarse-grained configurations are denoted by *f, g*, *h* and *k*, and they represent all real dimer configurations in which all 'internal' monomers on $G_r$ are black, while: in *f* all four corner monomers are black; in *g* two corner monomers (that belong to different sub-generators $G_{r-1}$, which are outlined by the dashed lines in coarse-grained generators in Figure 3) are black and the other two are white; in *h* two corner monomers (that belong to the same sub-generator $G_{r-1}$) are black and the other two are white; in *k* all four corner monomers are white. Other possible combinations of black and white corner monomers are not possible on this lattice. For example, combination of three black and one white and vice versa is not allowed because of the parity. Also, one can perceive that all close-packed dimer configurations, on generator of any order, belong to the coarse-grained configuration of the type *f*, while other three types are supplementary.

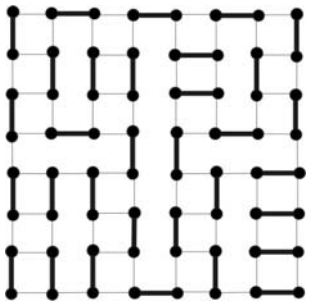

*Figure 2. Close-packed dimer configuration on the 5-th order generator of MR fractal lattice*

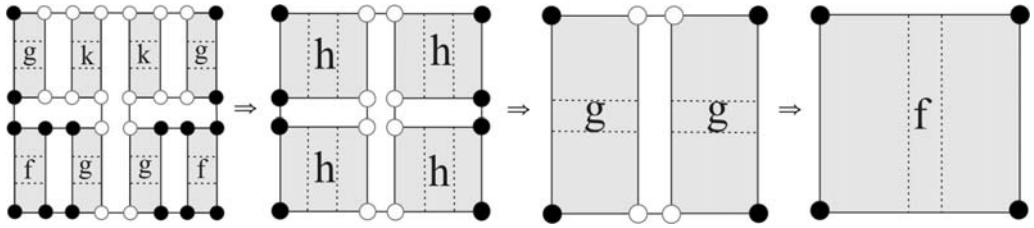


*Figure 3. Subsequent stages of coarse-graining procedure and designation of the coarse-grained configurations*

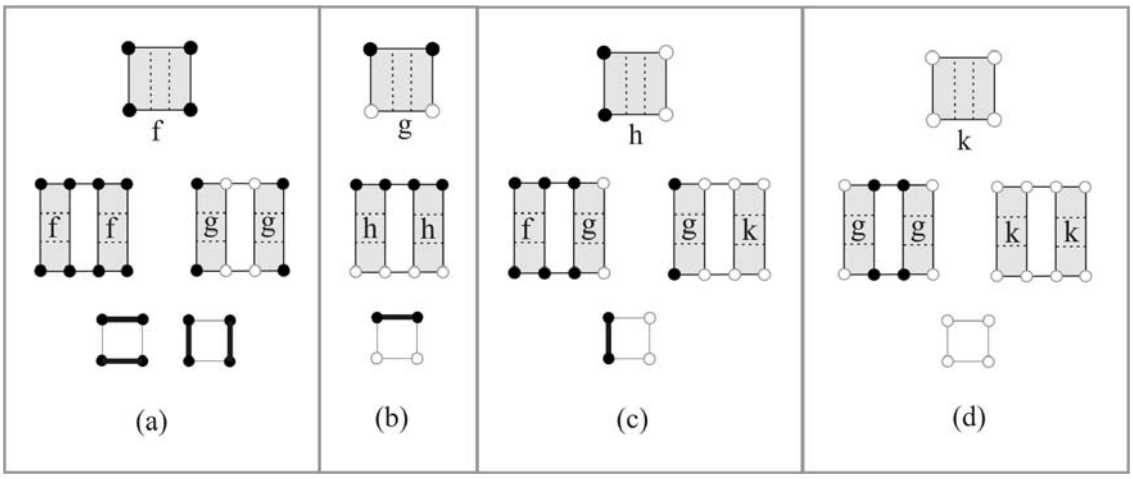


*Figure 4. Illustration of recursion relation formation and possible configurations on the unit square as the initial conditions that supplement recursion relations*

Due to the hierarchically constructed lattice, each of the four coarse-grained configurations on the $r$+1-th order generator, can be composed of the configurations of the same type on the $r$-th order generators. In the first row of Figure 4, we give schematic representation of four possible types of coarse-grained configurations. In the second raw, we illustrate how each of these configurations on the $r$+1-th order generators can be composed of configurations on the sub-generators. In Figure 4 (a), one can see how $f$ -type configuration on $G_{r+1}$ can be composed from either two $f$- type configurations on $G_r$ or two $g$-type configurations on $G_r$ . Denoting by $f_r$ all possible real close-packed dimer configurations on $G_r$ , and taking into account that every dimer configuration of type $f$ on one of the $G_r$ can be concatenated with every configuration of type $f$ on the second $G_r$ into one configuration on $G_{r+1}$ , we obtain $f_r^2$ close-packed dimer configurations. Similarly, from two $g$–type coarse-grained configurations on two sub-generators $G_r$ one can obtain $g_r^2$ close-packed dimer configurations on $G_{r+1}$ . The number of all close-packed dimer configurations on $G_{r+1}$ is then the sum of these two terms, and following the illustrations given in Figure 4 (b), 4(c) and 4(d) , one can write down recurrence equations:

$$f_{r+1} = f_r^2 + g_r^2 , \tag{1}$$

$$g_{r+1} = h_r^2 , \tag{2}$$

$$h_{r+1} = f_r g_r + g_r k_r , \tag{3}$$

$$k_{r+1} = g_r^2 + k_r^2 . \tag{4}$$

All possible dimer arrangements on the first order generator for each type of the configuration are shown in the third row in Figure 4 and represent initial values of the variables: $f_1 = 2$ , $g_1 = 1$ , $h_1 = 1$ and $k_1 = 1$.

Iterating recursion relations (1)-(4), starting from their initial values, the explicit numbers of close-packed dimer configurations on $G_r$ can in principle be obtained for any $r$. In Table 1, we present values of $f_r$ on several consecutive MR generators. As one can see from Table 1, the numbers of close-packed dimer configurations grow very fast with the lattice size, i.e. generator order $r$. In order to determine functional dependence of $f_r$ on $r$, the system of difference equations (1)-(4) should be solved. To accomplish this, we introduce new variables defined as: $x_r = g_r / f_r$ , $y_r = h_r / f_r$ and $z_r = k_r / f_r$ , whose recurrence equations follow from equations (1)-(4) and are given by:

$$x_{r+1} = \frac{y_r^{\,2}}{1 + x_r^{\,2}} , \tag{5}$$

$$y_{r+1} = \frac{x_r (1 + z_r)}{1 + x_r^{\,2}} , \tag{6}$$

$$z_{r+1} = \frac{x_r^{\,2} + z_r^{\,2}}{1 + x_r^{\,2}} . \tag{7}$$

In new variables, equation (1) can be written as:

$$f_{r+1} = f_r^{\,2} (1 + x_r^{\,2}) . \tag{8}$$

*Table 1. The numbers of close-packed dimer configurations $f_r$ on the first six generators of MR lattice ($f_1 = 2$).*

| order of generator | r=2 | r=3 | r=4 | r=5 | r=6 |
|---|---|---|---|---|---|
| $f_r$ | 5 | 26 | 757 | 575450 | 337201923781 |

Initial values for the variables $x$, $y$ and $z$ are given by $x_1 = y_1 = z_1 = 1/2$. Iterating recursion equations (5)-(7) we obtain that all three variables tend to zero (forming two monotonically decreasing sequences: one for odd *r* and one for even *r*, for each of the variables) when *r* tends to infinity. Since $x_r$ becomes negligibly small for $r >> 1$, the asymptotic form of equation (8) can be written as:

$$f_{r+1} \sim f_r^2,$$

which means that *f* grows exponentially with $2^r$. Assumed asymptotic form for $f_r$ is :

$$f_r \sim \omega^{2^r}, \tag{9}$$

where the growth constant $\omega$ can be obtained from

$$\ln \omega = \lim_{r\to\infty} \frac{\ln f_r}{2^r}.$$

Introducing the sequence $s_r = (\ln f_r)/2^r$, from equation (8) one obtains the recurrence relation

$$s_{r+1} = s_r + \frac{1}{2^{r+1}} \ln(1 + x_r^2), \tag{10}$$

with $s_1 = (\ln f_1)/2 = (\ln 2)/2$. Iterating recursion relation (10), together with relations (5)-(7), it is found that evaluated sequence of numbers converges very quickly, and its limiting value is equal to $s = \ln \omega = 0.414750739...$. Since the number of monomers is given by the number of lattice points, which is $N_r = 2^{r+1}$ for generator of order *r*, and the number of dimers $M_r$ is just a half of the number of monomers, equation (9) can be written as a function of $N_r$ or $M_r$ as:

$$f_r \sim (\sqrt{\omega})^{N_r}, \tag{11}$$

or

$$f_r \sim \omega^{M_r}. \tag{12}$$

From the known number of all close-packed dimer configurations, one can obtain the entropy as $S = k_B \ln f$. Setting the Boltzmann constant equal to unity, it follows from equation (12) that the entropy per dimer in the thermodynamic limit, i.e. $\lim_{M\to\infty} \frac{S}{M}$, is equal to the logarithm of the growth constant $\omega$, that is to $s = 0.414750739...$. Finally, the entropy per monomer is one-half of the entropy per dimer.

## 3. RESULTS AND DISCUSSION

In this paper, we have studied the close-packed dimer model on the modified rectangular (MR) fractal lattice. Enumerating the configurations recursively, we were able to find out explicit numbers of all close-packed dimer configurations on MR generator of any order *r*. Furthermore, we have determined the asymptotic form for the number of configurations as a function of the number of lattice sites. As can be seen from expression (11), the asymptotic form is a simple exponential function without any correction factors. Entropy per dimer is obtained from the overall number of configurations and its value can be compared to the result obtained for square lattice. This comparison is reasonable since MR lattice can be viewed as a square lattice from which some bonds are deleted. Each vertex in a square lattice has degree four (except boundary vertices for open boundary condition), i.e. there are four bonds (edges) attached to each vertex, while MR lattice vertices have degree three. This means that square lattice has much more bonds than MR lattice of the same size and, consequently, there are more possibilities to place dimers on the square lattice. This geometrical factor reflects on the entropy per dimer, which is $s_{sq} = 0.583121808...$ for the square lattice with both open and periodic boundary conditions [2], larger than $s_{MR} = 0.414750739...$ for MR lattice, as expected.

Finally, we would like to point out that there are many opportunities with this model for future work. It would be a challenging combinatorial problem to establish recurrence equations on the whole family of MR lattices [25]. Also, the model can be extended by introducing the interaction weights or even monomer-dimer problem can be considered on fractal lattices.

## 4. ACKNOWLEDGMENT

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## ПРЕБРОЈАВАЊЕ ДИМЕРНИХ КОНФИГУРАЦИЈА НА ФРАКТАЛНОЈ РЕШЕТКИ

**Сажетак:** У овом раду презентујемо рјешење за проблем потпуно пакованих димера на фракталној решетки. Димер модел се сматра изворним моделом статистичке физике који се може повезати са многим физичким појавама. Првобитно је уведен као модел за адсорпцију двоатомних молекула на површима. Овдје подразу-

мијевамо да је дводимензионални супстрат на коме се дешава адсорпција нехомоген и репрезентујемо га модификираном правоугаоном (МП) решетком. Самосличност фрактална решетке омогућава егзактно рекурентно пребројавање свих густо паковаих димерних конфигурација на сваком нивоу конструкције фрактална решетке. Одређен је асимптотски облик укупног броја димерних покривача и добијена је ентропија по димеру у термодинамичком лимесу.

**Кључне ријечи:** димерне конфигурације, адсорпција, фрактали, ентропија.