# Recurrence solution of monomer-polymer models on two-dimensional rectangular lattices 

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#### Abstract

The problem of counting polymer coverings on the rectangular lattices is investigated. In this model, a linear rigid polymer covers $k$ adjacent lattice sites such that no two polymers occupy a common site. Those unoccupied lattice sites are considered as monomers. We prove that for a given number of polymers ( $k$-mers), the number of arrangements for the polymers on two-dimensional rectangular lattices satisfies simple recurrence relations. These recurrence relations are quite general and apply for arbitrary polymer length $(k)$ and the width of the lattices $(n)$. The well-studied monomer-dimer problem is a special case of the monomer-polymer model when $k=2$. It is known the enumeration of monomer-dimer configurations in planar lattices is \#P-complete. The recurrence relations shown here have the potential for hints for the solution of long-standing problems in this class of computational complexity.


## 1 Introduction

The study of the combinatorial problem of enumerations of rigid rodlike molecules on lattices has a long history and has attracted interests from researchers in diverse fields of physics, mathematics, and theoretical computer
science. The system has been studied as a prototypical model for phase transitions in equilibrium statistical mechanics [26, 7, 39, 10, 4, 28. In this model, a linear rigid polymer covers $k$ adjacent lattice sites such that no two polymers occupy a common site. The polymers are usually called $k$-mers, and those unoccupied lattice sites are considered as monomers.

When $k=2$, the model becomes the well-studied monomer-dimer model. In 1961 a special case of the monomer-dimer model, the close packed dimer problem where the lattice is fully covered by dimers, was solved analytically [15, 5, 32]. It was further shown that counting dimer coverings of any planar lattices can be solved using the same Pfaffian method [16]. For the general monomer-dimer problem where unoccupied lattice sites (monomers) are allowed, no solution has been found despite decades of efforts [3, 9, 12, 30, 11, 33, 17, 38, 13, 21, 19, 20, 22, 1, 27. The importance of monomerdimer problem also comes from the fact that various other statistical physics problems can be mapped to the monomer-dimer model [16, 6, 23]. Solution of the monomer-dimer problem will lead to the solution of these other problems. For example, the Ising model in the absence of an external field, which was solved by Onsager in 1944 [25] using complicated methods, is mapped to the close packed dimer model, while in the presence of an external field it is mapped to the general monomer-dimer model. The model also acts as the classical limit of the recently introduced quantum dimer model which has been investigated intensively as the central model in modern theories of strongly correlated quantum matter [29].

The two-fold dichotomy of computational complexity of the monomerdimer problem, for counting dimer coverings of a planar lattice and a nonplanar lattice, as well as for counting close packed dimer configurations and counting coverings with nonzero monomers, has garnered the interest of researchers in theoretical computer science [14, 34, 35]. It has been shown that the enumeration of monomer-dimer configurations in planar lattices is \#Pcomplete [14], which indicates the problem is computationally "intractable". The class \#P plays the same role for counting problems (such as counting dimer configurations) as the more familiar NP class does for decision problems (such as the well-known satisfiability problem) [8, 2, 37, 24, 36]. The \#P-complete problems are at least as hard as the NP-complete problems in computational complexity hierarchy. If any problem in the \#P-complete class is found to be solvable, every problem in \#P class is solvable. Currently "P versus NP" problem is perhaps the major outstanding problem in theoretical computer science.

In this paper we give recurrence solutions of monomer-polymer models on two-dimensional rectangular lattices. These recurrence relations are quite general and apply for arbitrary polymer length $(k)$ and the width of the lattices $(n)$. The paper is organized as the follows. The major result is the Theorem 1 in Section 2. The proof of the theorem is given in Section 3. The methods used in the proof are elementary. In Section 4 the implications of the results are discussed.

## 2 Recurrence for the number of $k$-mers coverings

Consider a $n \times m$ two-dimensional rectangular lattice with $n$ lattice sites in the horizontal direction and $m$ lattice sites in the vertical direction. In the horizontal direction two kinds of boundary conditions will be considered: free boundary condition and cylinder boundary condition. In the latter case the lattice sites in the $n$th column are wrapped back and linked to the lattice sites in the first column. In the vertical direction only free boundary conditions will be considered.

Let $s$ denote the number of $k$-mers in the lattice, and denote the number of configurations of the $s k$-mers on a lattice with a width of $n$ and a length of $m$ by $a(k, n, m, s)$. Since $k, n$ and $s$ are fixed, in the following $a(k, n, m, s)$ is abbreviated as $a_{m, s}$ or $a_{m}$ for brevity. In the following the notation $\binom{p}{q}$ is used for the binomial coefficient of $p$ choose $q$.

The main result is stated in the following theorem:
Theorem 1 (Recurrence). For given $k, n$ and $s$, the following recursive relation holds:

$$
\begin{equation*}
\sum_{i=0}^{s}(-1)^{i}\binom{s}{i} a_{m-i, s}=c(n, k)^{s}, \quad m \geq k s \tag{1}
\end{equation*}
$$

where $c(n, k)$ is a constant that depends on the boundary conditions as well as $n$ and $k$, but not $m$ or $s$. For free boundary condition,

$$
c(n, k)= \begin{cases}2 n-k+1, & n \geq k \\ n, & n<k\end{cases}
$$

For cylinder boundary condition,

$$
c(n, k)= \begin{cases}2 n, & n \geq k \\ n, & n<k\end{cases}
$$

From Theorem 1 we can obtain the following recurrence:
Corollary 2 (Another recurrence).

$$
\begin{equation*}
\sum_{i=0}^{s+1}(-1)^{i}\binom{s+1}{i} a_{m-i, s}=0, \quad m \geq k s+1 \tag{2}
\end{equation*}
$$

Proof. Eq. (22) can be derived from Eq. (1): substitute $m-1$ into $m$ in Eq. (11), and subtract the two equations:

$$
\begin{aligned}
& a_{m}-\left[\binom{s}{1}+\binom{s}{0}\right] a_{m-1}+\cdots+(-1)^{s}\left[\binom{s}{s}+\binom{s}{s-1}\right] a_{m-s}-(-1)^{s} a_{m-1-s} \\
= & a_{m}-\binom{s+1}{1} a_{m-1}+\binom{s+1}{2}-\cdots+(-1)^{s}\binom{s+1}{s}-(-1)^{s} a_{m-1-s} \\
= & 0 .
\end{aligned}
$$

In above the following binomial identity is used:

$$
\begin{equation*}
\binom{j+1}{i}=\binom{j}{i}+\binom{j}{i-1}, \quad i>0 . \tag{3}
\end{equation*}
$$

To illustrate the recurrence stated in Theorem 1, some examples for different values of $k$ are listed in Table 1. In the table, $n=7, s=3$, and $m=20$. The lattices have free boundary conditions. The $k$-mer lengths take the range of $2,3,4,5$. The numbers are computed by extending the methods originally developed for the monomer-dimer problem $(k=2)$ to handle arbitrary lengths of $k$-mers [18, 19, 20, 21, 22].

For example, when $k=3$, we have
$1644154-\binom{3}{1} 1383884+\binom{3}{2} 1152702-948880=1728=(2 \times 7-3+1)^{3}$.

Table 1: The numbers $a_{m, s}$ for different $k$, with $n=7, s=3$, and $m=20$, on lattices with free boundary.

|  | $m$ |  |  |  |
| :--- | :--- | :--- | :--- | :--- |
| $k$ | 17 | 18 | 19 | 20 |
| 2 | 1491126 | 1788970 | 2124072 | 2498629 |
| 3 | 948880 | 1152702 | 1383884 | 1644154 |
| 4 | 560552 | 692133 | 843008 | 1014508 |
| 5 | 305326 | 384872 | 477398 | 583904 |

## 3 Proof of the recurrence

First we define the possible states of a $k$-mer covering a given lattice site. Notice that for a given lattice site, there are $k+2$ configurational states for a $k$-mer. The monomer state, where the lattice site is empty, is denoted as state 0 ; When the lattice site is occupied by the first part of the $k$-mer (in the positive $m$ direction), we say the $k$-mer is in state 1 for the given lattice site, and so on. When the last part of the $k$-mer occupies the lattice site, it's in state $k$. If the lattice site is occupied by a horizontal $k$-mer, a state $k+1$ is assigned. Figure 1 shows the 5 states for a trimer $(k=3)$. Note that the states are specific for a lattice site in a given row: if the $k$-mer is in a state $j$ for a lattice site in the $i$ th row, then it is in state $j-1$ for the site of the $(i+1)$ th row,

For proving the recurrence, we need to define certain numbers that count $k$-mer configurations with some $k$-mers restricted to given rows. Let $a_{\left(p_{1}, p_{2}, \cdots\right) m, s}^{\left(q_{1}, q_{2}, \cdots\right)}$ denote the number of configurations to have $s k$-mers in a $n \times m$ lattice with the requirement that at least one $k$-mer touching the $p_{1}$ th row from above (and none from below), at least one $k$-mer touching the $p_{2}$ th row from above (and none from below), etc., and at least one $k$-mer touching the $q_{1}$ th row from below (and none from above), at least one $k$-mer touching the $q_{2}$ th row from below (and none from above), etc.. For those $k$-mers restricted in the subscript of this notation, the $k$-mers are in the states of $k$ or $k+1$ with respect to the $p_{i}$ th row, while those $k$-mers restricted in the superscript are in the states of 1 or $k+1$ with respect to the $q_{i}$ th row.

Furthermore, another notation will be introduced: if the numbers $p_{i}$ in the subscripts have a bar, it means that there is at least one $k$-mers with state in the set $\{1,2, \ldots, k-1\}$ with respect of the $p_{i}$ th row of the lattice:


Figure 1: The configurational states of one $k$-mer on one lattice site. For a given lattice site each $k$-mer can have $k+2$ states. Here is an example for $k=3$. For the circled center site, the trimer can have 5 states: (a) state 0 : the site is empty; (b) state 1: the site is occupied by the first part of a vertical trimer; (c) state 2: the site is occupied by the middle part a vertical trimer; (d) state 3: the site is occupied by the end part a vertical trimer; (e) state 4 : the site is occupied by a horizontal trimer.
$a_{\left(p_{1}, p_{2}, \cdots, \overline{p_{i}}, \cdots\right) m, s}^{\left(q_{1}, q_{2}, \cdots\right)}$.
In the proof below, we only need $p_{i}$ 's to be in the rows of the set $\{1, k+$ $1,2 k+1, \ldots$,$\} , and q_{i}$ 's to be the last row, i.e., the $m$ th row. Hence the notation under these conditions becomes $a_{(1, k+1,2 k+1, \cdots) m, s}^{(m)}$. For brevity, a shorthand version will be used, which only uses the coefficients of $k$ in the subscripts:

$$
a_{(0,1,2, \cdots) m, s}^{(m)},
$$

and

$$
a_{(0,1,2, \cdots, \bar{i}, \cdots) m, s}^{(m)} .
$$

The sum of the numbers of rows in the subscript and superscript within the parentheses is the number of restricted $k$-mers. The rest of the $k$-mers can be arranged freely on the lattice (but not in contradiction to those restricted rows). Note that by symmetry, the superscript and subscript can be switched in totality without affecting the value. With these definitions, we first prove
the following lemmas. The proof of the recurrence in Theorem 1 is based on the following three lemmas.

The first lemma converts the difference between the enumerations of a lattice with a length $m$ and a lattice with a length $m-1$ to an enumeration with restrictions on the last row.
Lemma 2.1 (Go to the top).

$$
\begin{equation*}
a_{(0,1,2, \cdots, t) m, s}-a_{(0,1,2, \cdots, t) m-1, s}=a_{(0,1,2, \cdots, t) m, s}^{(m)}, \tag{4}
\end{equation*}
$$

where the coefficients in the subscripts within the parentheses of the three terms are the same, and can have bars over them.
Proof. Among all the $k$-mers configurations counted by $a_{(0,1,2, \ldots) m, s}$, some configurations have one or more $k$-mers touching the last row. These configurations are counted by $a_{(0,1,2, \cdots) m, s}^{(m)}$. For the rest of configurations none of the $k$-mers cover any sites of the last row: the last row is empty (unoccupied by $k$-mers). This is equivalent to a lattice of length $m-1$, hence the number of these configurations is counted by $a_{(0,1,2, \cdots) m-1, s}$.

The second lemma converts an enumeration with restrictions on the last row (the $m$ th row) to a sum of two terms: one term with the restrictions on the last row moved to the restrictions on a row at the bottom of the lattice that are $k$ sites above the topmost previously restricted row (the $[(t+1) k+1]$ th row), and the other term is with the barred version on the same row, but with the restriction on the last row unchanged.
Lemma 2.2 (Go to the bottom).

$$
\begin{align*}
& a_{(0, \ldots, t) m, s}^{(m)}=a_{(0, \ldots, t, t+1) m, s}+a_{(0, \ldots, t, \overline{t+1}) m, s}^{(m)}  \tag{5}\\
& a_{(0, \ldots, \bar{t}) m, s}^{(m)}=a_{(0, \ldots, \bar{t}, t+1) m, s}+a_{(0, \ldots, \bar{t}, \overline{t+1}) m, s}^{(m)} \tag{6}
\end{align*}
$$

Proof. For these $k$-mers configurations counted by $a_{(0, \ldots, t) m, s}^{(m)}$, consider the $((t+1) k+1)$ th row. The row can be empty, or if there are $k$-mers that intersect with this row, either they only have states in the set of $\{k, k+1\}$ on this row, or there exists at least one $k$-mer that is of state $\{1, \ldots, k-1\}$. For the former case (empty or in the states of $\{k, k+1\}$ ), we can fip the lattice between the $((t+1) k+1)$ th row and the $m$ th row, and the number of configurations in the flipped lattice are counted as $a_{(0, \ldots, t, t+1) m, s}$. The rest of the configurations are counted by $a_{(0, \ldots, t, \overline{t+1}) m, s}^{(m)}$. Similar arguments can be used for the second equation.

In the following we use $a_{(0, \ldots, t) m}^{(m)}(j)$ to emphasize that there are $j k$-mers that are not restricted to the rows specified by the subscripts or the superscript, with $t+2+j=s$.

Lemma 2.3 ( $j$ unrestricted $k$-mers).

$$
\begin{align*}
& \sum_{i=0}^{j+1}(-1)^{i}\binom{j+1}{i} a_{(0, \ldots, t) m-i, s}^{(m-i)}(j)=0  \tag{7}\\
& \sum_{i=0}^{j+1}(-1)^{i}\binom{j+1}{i} a_{(0, \ldots, t) m-i, s}^{(m-i)}(j)=0 \tag{8}
\end{align*}
$$

where $j$ stands for the number of unrestricted $k$-mers, with $t+2+j=s$, and $m \geq k s+1$. Similar identities also hold for $a_{(0, \ldots, t) m-i, s}$ and $a_{(0, \ldots, t) m-i, s}$, where there is no restriction on the last row. In these cases $t+1+j=s$.

Proof. These identities can be proved by mathematical induction. For $j=0$ the identities are true trivially: all $s k$-mers are constrained in the first $s-1$ rows and the last row, with one and only one $k$-mer intersect with each row, hence

$$
\begin{aligned}
& a_{(0, \ldots, t) m}^{(m)}(0)-a_{(0, \ldots, t) m-1}^{(m-1)}(0)=0, \\
& a_{(0, \ldots, t) m}^{(m)}(0)-a_{(0, \ldots, t) m-1}^{(m-1)}(0)=0 .
\end{aligned}
$$

Assume the identities are true for $j-1$, then for $j$ unrestricted $k$-mers we can use Lemma 2.1 and Lemma 2.2.

$$
\begin{aligned}
& \sum_{i=0}^{j+1}(-1)^{i}\binom{j+1}{i} a_{(0, \ldots, t) m-i}^{(m-i)}(j) \\
= & \sum_{i=0}^{j}(-1)^{i}\binom{j}{i}\left[a_{(0, \ldots, \bar{t}) m-i}^{(m-i)}(j)-a_{(0, \ldots, \bar{t}) m-i-1}^{(m-i-1)}(j)\right] \\
= & \sum_{i=0}^{j}(-1)^{i}\binom{j}{i}\left[\left[a_{(0, \ldots, \bar{t}, t+1) m-i}(j)+a_{(0, \ldots, \bar{t}, \overline{t+1}) m-i}^{(m-i)}(j-1)\right]\right. \\
& \left.-\left[a_{(0, \ldots, \bar{t}, t+1) m-i-1}(j)+a_{(0, \ldots, \bar{t}, \bar{t}+1) m-i-1}^{(m-i-1)}(j-1)\right]\right] \\
= & \sum_{i=0}^{j}(-1)^{i}\binom{j}{i}\left[a_{(0, \ldots, \bar{t}, t+1) m-i}^{(m-\bar{i})}(j-1)+a_{(0, \ldots, \bar{t}, t+1) m-i}^{(m-i)}(j-1)-a_{(0, \ldots, \bar{t}, \overline{t+1}) m-i-1}^{(m-i-1)}(j-1)\right] .
\end{aligned}
$$

In the first step the binomial identity Eq. (3) is used. In the second step Lemma 2.2 is used, and in the third step Lemma 2.1 is used. The three summands in the last sum all have $j-1$ unrestricted $k$-mers, and by the assumption their sums all vanish.

The second identity Eq. (8) and the identities without superscripts can be proved similarly.

Note that when $j=s$, Eq. (22) is obtained by using the identities of Lemma 2.3 without superscripts.

Finally, the recurrence of Eq. (11) in Theorem[1] can be proved. In the proof the following steps are used repetitively, reducing the number of unrestricted $k$-mers by one in each iteration: the binomial identity Eq. (3) is used to write the summand into a difference of two terms (Eq. (10) and Eq. (12)), Lemma 2.1 is then used to convert the difference of the two terms into one term by introducing the restriction to the top row (Eq. (11) and Eq. (13), where in Eq. (11) $\left.a_{(0) m-i}=a_{m-i}^{(m-i)}\right)$, thus reducing the number of unrestricted $k$-mers by one. The Lemma 2.2 is then used to bring this restriction on the top row to the bottom (Eq. (14)), releasing the constraints on the top row so that Lemma 2.1] can be applied again in the next iteration. In doing so this step introduces an extra term with a bar in the subscripts. Then Lemma 2.3 is used to make the sum of this extra term vanish (Eq. (15)). After one iteration of these steps, the number of unrestricted $k$-mers is reduced by one. In the final step, only one term remains, where the restrictions are on bottom $s$ rows of the lattice, with the rows indexed as: $1, k+1,2 k+1, \ldots,(s-1) k+1$, each separated from the next by a length of $k$. Thus the $s k$-mers can be arranged on these $s$ rows independently, leading to the final result.

## Proof of Theorem 1 .

$$
\begin{align*}
& \sum_{i=0}^{s}(-1)^{i}\binom{s}{i} a_{m-i}  \tag{9}\\
= & \sum_{i=0}^{s-1}(-1)^{i}\binom{s-1}{i}\left[a_{m-i}-a_{m-i-1}\right] \quad \text { by Eq. (3) }  \tag{10}\\
= & \sum_{i=0}^{s-1}(-1)^{i}\binom{s-1}{i} a_{(0) m-i} \quad \text { by Lemma 2.1] }  \tag{11}\\
= & \sum_{i=0}^{s-2}(-1)^{i}\binom{s-2}{i}\left[a_{(0) m-i}-a_{(0) m-i-1}\right] \quad \text { by Eq. (3) }  \tag{12}\\
= & \sum_{i=0}^{s-2}(-1)^{i}\binom{s-2}{i} a_{(0) m-i}^{(m-i)} \quad \text { by Lemma 2.1] }  \tag{13}\\
= & \sum_{i=0}^{s-2}(-1)^{i}\binom{s-2}{i}\left[a_{(0,1) m-i}+a_{(0, \overline{1}) m-i}^{(m-i)}\right] \quad \text { by Lemma [2.2 }  \tag{14}\\
= & \sum_{i=0}^{s-2}(-1)^{i}\binom{s-2}{i} a_{(0,1) m-i} \quad \text { by Lemma 2.3 }  \tag{15}\\
= & \cdots  \tag{16}\\
= & a_{(0,1, \ldots, s-1) m}=c(n, k)^{s} . \tag{17}
\end{align*}
$$

In the last step, the $s k$-mers are in $s$ rows of the lattice that are $k$ sites apart, so their configurations are independent of each other. The number of arrangements for one $k$-mer in a lattice strip of $n \times k$ is denoted by $c(n, k)$. For the free boundary condition, when $n \geq k$,

$$
c(k, n)=(n-k+1)+n=2 n-k+1
$$

where the terms within parenthesis is for the $k$-mer in horizontal orientation, and the last term $n$ is for the $k$-mer in vertical orientation. When $n<k$, the first term does not exist and $c(k, n)=n$.

For the cylinder boundary condition, when $n \geq k$, there are $n$ configurations for the $k$-mer in horizontal orientation, and $n$ configurations in vertical orientation, so $c(k, n)=2 n$. When $n<k, c(k, n)=n$ for vertical orientation only, as in the case of the free boundary condition.

## 4 Concluding remarks

The recurrences of Eq. (11) and Eq. (2) show that the enumerations of monomerpolymer coverings in two-dimensional lattices have some regular patterns. From the recurrences we can obtain the generating function for the number of coverings for a lattice with width $n$ and a fixed number of $k$-mers of $s$ in the form of 31]

$$
G(x ; k, n, s)=\sum_{m=0}^{\infty} a_{m, s} x^{m}=\frac{c(n, k)^{s} x^{k s}}{(1-x)^{s+1}}+\frac{P(x ; k, n, s)}{(1-x)^{s}}
$$

where $P(x ; k, n, s)$ is a polynomial in the indeterminate variable $x$ with a degree of $k s-1$. The polynomial $P(x ; k, n, s)$ is determined by the initial conditions of the recurrences. The generating function has only one pole at $x=1$ with a multiplicity of $s+1$. The expansion of the first term by the binomial theorem gives

$$
c(n, k)^{s}\binom{m+s-k s}{s}
$$

as the contribution to $a_{m, s}$ from the first team, but the expansion of the second term depends on the polynomial $P(x ; k, n, s)$. It would be interesting to find out what kinds of patterns the polynomial $P(x ; k, n, s)$ has and how they contribute to the enumerations of monomer-polymer coverings.

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