Computing the monomer-dimer systems through matrix permanent

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The monomer-dimer model is fundamental in statistical mechanics. However, it is \#P-complete in computation, even for two dimensional problems. A formulation in matrix permanent for the partition function of the monomer-dimer model is proposed in this paper, by transforming the number of all matchings of a bipartite graph into the number of perfect matchings of an extended bipartite graph, which can be given by a matrix permanent. Sequential importance sampling algorithm is applied to compute the permanents. For two-dimensional lattice with periodic condition, we obtain $0.6627 \pm 0.0002$, where the value is $h_2 = 0.662798972834$. For three-dimensional problem, our numerical result is $0.7847 \pm 0.0014$, which agrees with the best known bound.

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I. INTRODUCTION

The monomer-dimer model is considered, in which the set of sites in a lattice is covered by a non-overlapping arrangement of monomers (molecules occupying one site) and dimers (molecules occupying two sites that are neighbors in the lattice). It is fundamental in lattice statistical mechanics \([1, 2]\). A two dimensional monomer-dimer model with size $m = (m_1, m_2)$ is a rectangle lattice with $m_1 \times m_2$ sites. The two dimensional monomer-dimer systems are used to investigate the properties of adsorbed diatomic molecules on a crystal surface \([3]\); the three-dimensional systems occur classically in the theory of mixtures of molecules of different sizes \([4]\) as well as the cell cluster theory of the liquid state \([5]\). More complete description of the history and the significance of monomer-dimer model can be found in \([1]\) and the references therein.

All possible monomer-dimer coverings for a given lattice defines the configuration space of a monomer-dimer model. A fundamental question for such a statistical mechanics model is to determine the cardinal number of the configuration space. Practically, most of the thermodynamic properties of physical systems can be obtained from the number of all possible ways that a given lattice can be covered. Thus a considerable attention has been devoted to such a counting problem. For a d-dimensional cubic lattice with size $m = (m_1, m_2, \cdots, m_d)$, this cardinal number is denoted by $Z(m, d)$. It is proved that the following limit exists

$$h_d = \lim_{m \to \infty} \frac{\log Z(m, d)}{m_1m_2\cdots m_d}$$

The limit $h_d$ is called monomer-dimer constant \([6]\).

Even for the simplest two dimensional models, there are very few closed form results on the monomer-dimer constant. Baxter and Gaunt \([8, 9]\) gives estimates of the constants using the asymptotic expansions. Hammersley and Menon \([10]\) estimate the $h_2$ by calculating lower and upper bounds. Numerical simulation should play a very important role. However it has been proved that computing the monomer-dimer constant is a \#P-complete problem even for 2-dimensional problems \([10]\), which shows the hardness of the computation. The Monte Carlo method is applied to study the problem in \([2, 6, 11]\), which is a natural consideration. Recently, Friedland and Peled \([12]\) give a complete up-to-date theory of the computation of monomer-dimer constant by calculating lower and upper bounds. They obtain $h_2 = 0.66279897$, which agrees with the heuristic estimation $e^{h_2} = 1.940215351$ due to Baxter \([2]\), and $0.7653 \leq h_3 \leq 0.7862$. Two-dimensional model with fixed dimer density is studied intensively by Kong \([13]\). The monomer-dimer constant with 12 digits accuracy for two dimensional problem is given as $h_2 = 0.662798972834$.

In this paper, we propose a formulation that transforms the counting of all matchings of a bipartite graph to the counting of perfect matchings of an extended bipartite graph. Hence, the monomer-dimer constants in any dimensions can be computed by permanents of matrices. Permanent of matrix is studied for a very long time \([14, 15]\). After Valiant proves that evaluating the permanent of a 0-1 matrix is a \#P-complete problem \([16]\), many randomized approximate algorithms are developed \([17, 18, 19]\). They can give reasonable estimations for permanent within an acceptable computer time.

We consider cubic lattice with periodic condition, and concentrate on two and three dimensional lattices in the computation. The algorithms are applicable to other dimensions and domains other than rectangle. For simplicity of notation, we assume that $m_1 = m_2 = \cdots = m_d$. But this is not essential for the algorithms.

In the next section, the formulation of the monomer-dimer configuration space in matrix permanent is presented. Computational methods are discussed in section III. The sequential importance sampling algorithms are given to compute matrix permanents. In section IV, numerical results are presented which clearly shows the efficiency of our formulation and the computational meth-
odds. Finally in section V, some discussions and comments are given.

II. FORMULATION IN PERMANENT

Consider each point/site in the lattice as a vertex, and an edge exists if the two vertices are neighbors in the lattice. Hence a graph \( G = (V, E) \) is naturally defined. Using the terminology of graph theory, a monomer-dimer system can be represented as a covering of the vertices of the graph \( G = (V, E) \) by a non-overlapping arrangement of monomers (molecules covering one vertex) and dimers (molecules covering a pair of adjacent vertices).

It is convenient to identify monomer-dimer configurations with matching in the graph \( G \). The sites of a cubic lattice can be divided into two vertex sets \( V_1 \) and \( V_2 \). A site and its neighbor should always belong to different vertex sets. There are edges between neighbors, and all edges form a edges set \( E \). Thus an undirected bipartite graph \( G(V_1 \cup V_2, E) \) is constructed. In terms of the graph theory, a covering of all vertices with dimers is a perfect matching of the bipartite graph \( G(V_1 \cup V_2, E) \); and a covering with \( k \) dimers is a \( k \)-matching of it. Hence the cardinal number of the configuration space of the monomer-dimer model equals to the number of all possible matchings of the bipartite graph \( G \).

The partition function of the system is defined as

\[
Z(\lambda) \equiv Z_G(\lambda) = \sum_{k=0}^{n} m_k \lambda^k
\]  

(1)

where \( m_k = m_k(G) \) is the number of \( k \)-matching in the graph \( G \), which is equivalent to the number of monomer-dimer configurations with \( k \) dimers. \( Z_G(1) \) enumerates all possible matchings in \( G \).

Let \( G \) be a bipartite graph and \( A \) be the adjacent matrix of the graph \( G \). The number of perfect matchings of \( G \) is equal to the permanent of the matrix \( A \), which is defined as

\[
\text{perm}(A) = \sum_{\sigma \in \Pi_n} \prod_{i=1}^{n} a_{\sigma(i)}.
\]  

(2)

Here \( \Pi_n \) is the symmetric group of degree \( n \).

A matrix permanent formulation for enumerating \( k \)-matching of a bipartite graph is proposed by Friedland and Levy recently \[21\]. Their method can be applied to approximate the monomer-dimer constant. For any given \( k \), method by Friedland and Levy can compute \( m_k \), the number of \( k \)-matching, for all \( k \in \{0,1,\ldots,n\} \). Thus \( Z_G(1), \) all possible matchings in \( G \), can be given by

\[
Z_G(1) = \sum_{k=0}^{n} m_k.
\]  

Note that the number of matrix permanents computed is \( n \), and \( n \) would not be a small number. Here in the following we propose a new formulation in matrix permanent. The number of all possible matchings, that is \( Z_G(1) \) in \( 3 \), can be approximated directly.

Let \( A \) be the adjacent matrix of a bipartite graph \( G \). Thus \( A \) is a 0-1 matrix. We use \( G(A) \) denote the bipartite graph with adjacent matrix \( A \). The vertex set of \( G(A) \) is denoted as \( V = V_1 \cup V_2 \) and the edge set is \( E \). An auxiliary graph is constructed based on graph \( G(A) \) as follows. Vertex sets \( V_1' \) and \( V_2' \) are added to \( V_1 \) and \( V_2 \) respectively. The cardinal numbers of the new sets \( V_1' \) and \( V_2' \) are both \( n \). There are \( n \) edges between \( V_1 \) and \( V_2 \) and each vertex in \( V_1 \) is adjacent to a different vertex in \( V_2' \). The vertexes of \( V_1' \) are adjacent to every vertexes of \( V_2 \) and \( V_2' \). Let

\[
B = \begin{pmatrix}
A & I_{n \times n} \\
1_{n \times n} & I_{n \times n}
\end{pmatrix},
\]  

(4)

where \( 1_{n \times n} \) is the \( n \times n \) matrix whose entries are all equal to 1; and \( I_{n \times n} \) is the identity matrix of order \( n \). It is obvious that \( B \) is a 0-1 matrix, and it is the adjacent matrix of the auxiliary graph.

Let \( AM(A) \) denote the number of all possible matchings of the graph \( G(A) \). Note that \( \text{perm}(B) \) gives the number of perfect matchings of \( G(B) \). In a perfect matching of \( G(B) \), each vertex \( V_1 \) is assigned to be adjacent to a vertex in \( V_2 \cup V_2' \). The number of all the possible assignment between \( V_1 \) and \( V_2 \cup V_2' \) equals to \( AM(A) \). If the adjacent edges between the set \( V_1 \) and set \( V_2 \cup V_2' \) are chosen, there are \( n! \) possibilities for choosing the adjacent edges between \( V_1 \) and \( V_2 \cup V_2' \). So we have \( AM(A) \cdot n! = \text{perm}(B) \), that is

\[
AM(A) = \frac{1}{n!} \text{perm} \begin{pmatrix}
A & I_{n \times n} \\
1_{n \times n} & I_{n \times n}
\end{pmatrix}.
\]  

(5)

Denote

\[
f(\lambda) = \frac{1}{n!} \text{perm} \begin{pmatrix}
A & \lambda \cdot I_{n \times n} \\
1_{n \times n} & I_{n \times n}
\end{pmatrix} = \sum_{k=0}^{n} f_k \lambda^k.
\]  

Let \( m_k = m_k(G(A)) \) be the number of \( k \)-matching in the graph \( G(A) \). It is easy to verify that,

\[
m_k = f_{n-k}.
\]  

(6)

Thus we can get the following permanent formulation of the partition function of monomer-dimer system.

\[
Z(\lambda) \equiv Z_G(\lambda) = \sum_{k=0}^{n} f_{n-k} \lambda^k.
\]  

(7)

Hence the partition function of the monomer-dimer system is formulated as matrix permanent. It is important to notice that the matrix \( B \) is very special in structure, which will be explored in the following numerical algorithms.
III. COMPUTATIONAL METHODS THROUGH PERMANENT

Matrix permanent is a long-studied mathematical problem in its own right [14, 15]. A bridge between the computation of permanent and monomer-dimer constant is established via the relationship [16]. Thus the monomer-dimer constant can be computed by taking the advantage of the efficient algorithms in matrix permanent.

The definition of the permanent $\text{perm}(A)$ looks similar to that of the determinant $\det(A)$. However it is much harder to be computed. Valiant [16] proves that computing a permanent is a $\#P$-complete problem in counting, even for 0-1 matrices. Hence approximate algorithms, which can give a reasonable estimation for $\text{perm}(A)$ within acceptable computer time, attract much attentions recently.

Practical approximate methods for matrix permanents are Monte Carlo algorithms. One way to do so is to relate matrix permanents to matrix determinants by randomizing the elements of matrices [17, 18]. The Markov chain Monte Carlo approach can give a fully polynomial randomized approximation scheme for the permanent of any arbitrary nonnegative matrix. This is obtained by M.Jerrum, A.Sinclair and E.Vigoda [19]. Beichl, O’Leary and Sullivan [20] compute the number of $k$-matching of monomer-dimer model using Markov chain Monte Carlo method. They improve the KRS method [2].

The Monte Carlo methods with sequential importance sampling, which are a kind of efficient algorithms for approximating permanent, seem to be promising for the monomer-dimer problem [20, 22, 23]. Beichl and Sullivan give the best known numerical result for 3-D dimer approximation scheme for the permanent of any arbitrary nonnegative matrix. This is obtained by M.Jerrum, A.Sinclair and E.Vigoda [19]. Beichl, O’Leary and Sullivan [20] compute the number of $k$-matching of monomer-dimer model using Markov chain Monte Carlo method. They improve the KRS method [2].

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Algorithm SIS-P

Step 1. Choose a nonzero element from the first row of the matrix $A$ with some probability $p_1$. Suppose the column index of this element is $k_1$. Set all the other entries in the first row and the $k_1$th column to 0’s;

Step 2. Proceed to the next row, applying the same sampling strategy as step 1 recursively. Hence the values $p_2, \ldots, p_n$ can be obtained;

Step 3. Compute $X = \frac{1}{p_1} \cdot \frac{1}{p_2} \cdot \ldots \cdot \frac{1}{p_n}$.

The output $X$ of Algorithm SIS-P is a random variable. It is an unbiased estimator to the permanent of 0-1 matrix $A$. Different strategies of choosing the probability distributions would lead to different sequential importance sampling algorithms.

Now we apply Algorithm SIS-P to compute the permanent of the matrix $B$ in [23]. The matrix structure is so special that all the elements in the $(n+1)$th to $(2n)$th rows of $B$ are 1. Hence only the first $n$ rows of $B$ are needed to be considered. Assume that one sampling gets probability values $p_1, p_2, \ldots, p_n$. The sampling value should be assigned as

$$\frac{1}{p_1} \cdot \frac{1}{p_2} \cdot \ldots \cdot \frac{1}{p_n} \cdot n!.$$

If $N$ samples are obtained by Algorithm SIS-P, the number of all matchings can be approximated by

$$\text{AM}(A) = \frac{\text{perm}(B)}{n!} \approx \frac{1}{p_1} \cdot \frac{1}{p_2} \cdot \ldots \cdot \frac{1}{p_n} \cdot \sum_{j=1}^{N} \frac{1}{p_1^{(j)}} \cdot \frac{1}{p_2^{(j)}} \cdot \ldots \cdot \frac{1}{p_n^{(j)}}.$$

Three different importance sampling methods Ras by [22], Liu by [20], and B-S by [23] are used respectively to compute the number of the cardinal number of the configuration space. The results are given in Table I. The convergence rates of the three algorithms for $m = 4$ are also shown in FIG. III. Simple examples show that both Liu and B-S give good results, and Liu runs faster in the computation of monomer-dimer constant.

According to the law of large numbers, the mean value of these samples gives an approximation to the permanent. But in fact, the number of samples in our computation is not really “large”. More precisely, a typical sample number in our computation would be 100,000, while the cardinal number of the sample space could be,

| m   | Ras value time(s) | Liu value time(s) | B-S value time(s) | exact value |
|-----|------------------|------------------|------------------|-------------|
| 2   | 6.9999 1.72      | 7.0000 1.99      | 7.0017 4.164     | 7           |
| 4   | 41225 8        | 41225 5.55      | 41985 19.47      | 41025       |

FIG. I: The lattice is a $(4, 4)$ lattice and thus the adjacent matrix is $16 \times 16$. The x-axis denotes the number of samplings and the y-axis denotes the error of the approximate cardinal number of configuration space.
for example, $10^{115}$ (the two dimensional monomer-dimer model with $m = 20$).

Notice that the probability distribution of the random variable $Y = \log X$ looks similar to the normal distribution. If the probability distribution of $Y$ is normal with $N(\mu, \sigma)$, then the expectation of $X$ would be

$$E(X) = E(e^{Y}) = e^{\mu + \sigma^2/2}.$$ 

Other than computing the sample mean of $X$ directly, we can estimate the sample mean $\bar{\mu}$ and sample standard deviation $\bar{\sigma}$ of the random variable $Y$ first.

### IV. EXPERIMENTAL RESULTS FOR PERIODIC LATTICES

The algorithm SIS is used to approximate permanents, which gives approximation to the monomer-dimer constants. The algorithms are programmed in Matlab 7.0 and all computations in this paper run on Dell PC with CPU 2.8G Hz.

#### A. Experiments on two dimensional lattices

Computational results for 2-dimensional monomer-dimer problems with periodic boundary conditions are presented in TABLE II.

| $m$ | SIS     | Time (sec) | A-PRE |
|-----|---------|------------|-------|
| 4   | 0.663866| 0.0012     | 0.6611|
| 6   | 0.662851| 0.0019     | 0.6629|
| 8   | 0.662897| 0.0028     | 0.6611|
| 10  | 0.662951| 0.0038     | 0.6663|
| 12  | 0.662990| 0.0055     | 0.6646|
| 14  | 0.662852| 0.0072     | 0.6638|
| 16  | 0.662644| 0.0100     | —     |
| 18  | 0.663390| 0.0138     | —     |
| 20  | 0.662960| 0.0181     | —     |
| 22  | 0.663031| 0.0237     | —     |
| 24  | 0.662893| 0.0307     | —     |
| 26  | 0.663754| 0.0398     | —     |
| 28  | 0.663013| 0.0507     | —     |
| 30  | 0.663062| 0.0710     | —     |
| 32  | 0.662587| 0.0769     | —     |

Let compare with the results and the algorithm A-PRE, a Markov Chain Monte Carlo method used by Beichl, O’Leary, and Sullivan[11]. Though computers used here are different, one can still tell the trends in the running times. The curve fitting results for algorithms SIS and A-PRE are shown in FIG 2. It is clear that the running times for both SIS and A-PRE grow polynomially with respect to $m$. The time complexity of SIS, the method developed in this paper, is about $O(m^3)$ for 2-dimensional lattice, while the A-PRE, the MCMC method by [11], is about $O(m^5)$. Hence it is easy to tell that the algorithm SIS is faster distinctly. This suggests that the method SIS can be applied to large monomer-dimer problems.

#### B. Experiments on three dimensional lattices

For 3-dimensional problem with periodic condition, computational results are shown in TABLE III. The time complexity for algorithm SIS in 3 dimensional problems is about $O(m^6)$.

In order to fit the limit of $\log Z(m, 2)/m^2$ as $m$ goes to infinity, we apply regression to the computed mean values. The regression function is the same as [23]

$$y = \frac{p_1}{x^2} + p_2,$$

where $x$ denotes the lattice size $m$, $y$ denotes the $h_2(m)$ and $p_2$ is the monomer-dimer constant. The monomer-dimer constant of 2-dimensional problem with periodic boundary can be obtained from the regression

$$h_2 = 0.6627 \pm 0.0002 \text{ with } 95\% \text{ confidence}.$$ 

The approximate results of the monomer-dimer constant coincides with the value $h_2 = 0.662798972834$ by [13] very well.
TABLE III: \( m \) denotes the size of the cubic \((m, m, m)\) lattice. Every time, we sample 100,000 samples and compute the approximate result of \( \log Z(m, 3)/m^3 \). We do this several times. SIS gives the median value of the approximate values; Time denotes the time in second for one sampling. A-PRE is the value given in [11].

| \( m \) | SIS     | Time(sec) | A-PRE  |
|--------|---------|-----------|--------|
| 4      | 0.787359| 0.0039    | 0.7844 |
| 6      | 0.786661| 0.0082    | 0.7847 |
| 8      | 0.785821| 0.0345    | 0.7870 |
| 10     | 0.787093| 0.0919    | —      |
| 12     | 0.785054| 0.2483    | —      |
| 14     | 0.783476| 0.6693    | —      |

To fit the limit of \( \log Z(m, 3)/m^3 \) as \( m \) goes to infinity, we apply regression again. The function we use is

\[
y = \frac{p_1}{x} + p_2, \tag{9}
\]

where \( x \) denotes the lattice size \( m \), \( y \) denotes the \( h_3(m) \) and \( p_2 \) is the monomer-dimer constant. The result is

\[
h_3 = 0.7847 \pm 0.0014 \text{ with } 95\% \text{ confidence.}
\]

This agrees well with the best known bound \( 0.7653 \leq h_3 \leq 0.7862 \) [12].

V. DISCUSSIONS AND COMMENTS

The construction of the auxiliary bipartite graph is the key step in our formulation. Hence the permanent of the matrix \( B \) in (4) gives the total number of matchings in the original bipartite graph \( G(A) \). The size of the matrix \( B \) doubles that of \( A \). However since the special structure of the matrix \( B \) can be explored in the algorithm, the computational cost does not really increase.

The Monte Carlo method we used in this paper is based on the sequential importance sampling. Each time one samples a term from the large sum defined by (2), and only nonzero terms are valuable in the computation. The formulation and computational methods that we propose in this paper never meet any zero term. This fact is not obvious but crucial for the efficiency of the algorithm. A rigorous mathematical proof will be presented elsewhere.

The regression function (8) for two dimensional is discussed and used by many authors, for example [23]. It is based on asymptotic analysis. However (9) for three dimensional is just a result of statistical experiments. We are unable to give it any physical reasoning.

The basic contribution of this paper is the formulation and computational methods for approximating the number of all matchings in bipartite graphs. In this way, larger monomer-dimer systems can be studied.

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