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Transfer matrix algorithm for computing the exact partition function of a square lattice polymer

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ABSTRACT

I develop a transfer matrix algorithm for computing the exact partition function of a square lattice polymer with nearest-neighbour interactions by extending a previous algorithm for computing the total number of self-avoiding walks. The computation time scales as $\sim 1.6^N$ with the chain length N, in contrast to the explicit enumeration where the scaling is $\sim 2.7^N$. The exact partition function can be obtained faster with the transfer matrix method than with the explicit enumeration for $N > 25$. The new results for up to $N = 42$ are presented.

1. Introduction

Polymers play important roles in various fields of science, including biology, where various biopolymers perform crucial functions for life processes. Although the properties of heteropolymers such as proteins are most interesting, many important general properties of polymers can be learned from simpler homopolymer models. The simplest toy models for studying such a polymer are lattice models, such as two-dimensional square or three-dimensional cubic lattice polymers [1–4]. By introducing hydrophobic inter-monomer interactions, a lattice model can be used as a model for a polymer in a dilute solution [1–30]. Various quantities such as the radius of gyration, end-to-end distance, and specific heat have been calculated for the lattice models.

One important advantage of the lattice polymer is that all the possible conformations can be enumerated exactly [29–32]. The exact partition function for lattice polymers up to $N = 28$ for cubic lattices and $N = 40$ for square lattices has been computed by a recently developed efficient enumeration algorithm [32], where N is the number of monomers in the polymer. The most serious obstacle for the explicit enumeration of lattice polymer conformations of longer chain lengths is the fact that the number of conformations and the corresponding computational time grows exponentially with the chain length, as $\sim 2.7^N$ [31,32].

In this work, I propose a new transfer matrix approach where the exact partition function of a square lattice polymer can be computed much faster than using the explicit enumeration for long chains. In the transfer matrix method, instead of generating one conformation at a time, one keeps track of an ensemble of partially built conformations. By discarding detailed information on the partially built conformations and retaining only the essential information required for the computation of the partition function, the transfer matrix method drastically reduces the computational time without sacrificing the exact nature of the computation. The transfer matrix approach has been mostly used for computing the partition function for spin systems [33,34], including a simple model of proteins [35,36]. The most relevant previous work is the transfer matrix method used for the enumeration of self-avoiding walks (SAWs) on the square lattice [37]. This method is an improvement of earlier methods for enumerating SAWs [38,39], and also an extension of the methods that enumerates the self-avoiding polygons (SAPs) on the square lattice [40–42]. Because a conformation of a lattice polymer is equivalent to a SAW, the *total* number of polymer conformations on the square lattice is enumerated by this method. The computation has been performed for up to $N = 80$ [37]. We generalize this method so that the nearest-neighbour contact between the monomers can be taken into account. By computing the number of conformations for each value of the contact number, the exact partition function can be computed as a function of the temperature. We find that the computational time scales as $\sim 1.6^N$, in contrast to $\sim 2.7^N$ of the explicit enumeration. The partition function can be obtained much faster with the transfer matrix method than with the explicit enumeration for $N > 25$. All the known results up to $N = 40$ can be reproduced within a day with a *single* CPU. The new results for $N = 41$ and $N = 42$ will also be presented.

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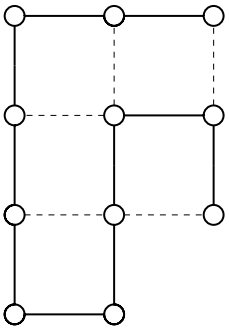

Fig. 1. Example of a conformation of a square lattice polymer, with $N = 11$ and $K = 5$. The non-bonded contacts are denoted by dashed lines.

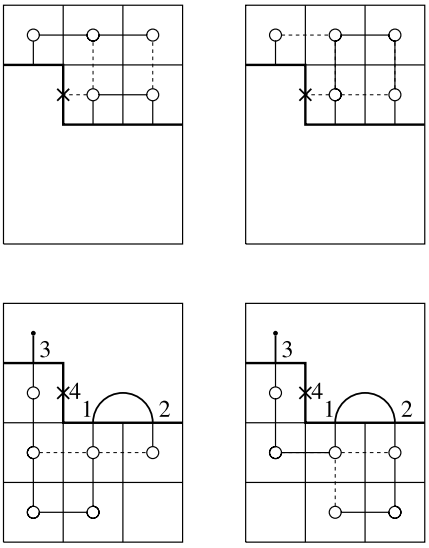

Fig. 2. Example of building polymer conformations of length $N = 11$ spanning the box of rectangle 3×4. The current cut-line is shown as the thick line. The cell at $(i, j) = (1, 3)$ has been just been completed, and the signature at the cut-line is (3 4 1 2). An empty edge with a cross on it denotes that the site just beneath the edge is occupied. Two examples of a partially built conformation with $n = 6$, $k = 2$, corresponding to this signature, are also shown below the cut-line at the bottom of the figure. Two examples of the upper parts of the conformations with $K = 5$, generated from this cut-line signature, are shown at the top.

2. Model

We consider a polymer on a square lattice, where a pair of non-bonded monomers that are neighbouring with each other is regarded as being in contact. The energy value of $-\epsilon$ is associated with each of these nearest-neighbour contacts. Therefore, the energy of a given conformation can be expressed as $E = -\epsilon K$, where K is the number of contacts formed in the conformation, which will simply be called the contact number from now on. An example of a square-lattice polymer conformation with $N = 11$ and $K = 5$ is shown in Fig. 1. The partition function is then given by

$$Z = \sum_{\text{all confs}} e^{-\beta E} = \sum_{K=0}^{K_{\max}} \Omega(K) e^{\beta \epsilon K}, \tag{1}$$

where $\beta \equiv 1/k_B T$ and $\Omega(K)$ indicate the number of conformations for a given contact number K, also called the density of states. For the polymer on the square lattice, the maximum number of possible contacts $K_{\max}$ is given as [1]:

$$K_{\max}(N) = \begin{cases} N - 2m & \text{for } m^2 < N \le m(m+1), \\ N - 2m - 1 & \text{for } m(m+1) < N \le (m+1)^2, \end{cases} \tag{2}$$

where m is a positive integer and N is the number of monomers forming the polymer chain. It is clear from Eq. (1) that the partition function for any temperature T can be computed once the density of states $\Omega(K)$ is obtained. The purpose of the algorithm developed in the current study is the efficient computation of $\Omega(K)$. The current model is also called the interacting self-avoiding walk (ISAW) on the square lattice. When $\beta = 0$, the partition function of ISAW in Eq. (1) gets reduced to the *total* number of SAWs that has been computed by the transfer matrix approach [37,38].

3. Transfer matrix method

The transfer matrix method developed in the current study is based on a previous method for enumerating the total number of SAWs on the square lattice [37]. First, the conformations are classified according to the rectangular box they span. For a given box, only the conformations touching all four walls of the box are enumerated. This idea has also been implemented in a parallel algorithm for explicit enumeration [31]. Let us denote the width and height of the box as w and h, respectively. It is convenient to visualize the box as consisting of $w \times h$ cells, with each cell enclosing a lattice site (Fig. 2). Because the conformation is required to touch all the walls of the box, we get the upper bound for the box size, $w + h - 1 \le N$. In fact, the number of conformations spanning the box with $w + h - 1 = N$ can be obtained with an analytic formula, so only the conformations spanning the boxes with $w + h - 1 < N$ need to be enumerated [31]. Because the polymer conformations must fit inside the box, there is also a lower bound $w \times h \ge N$.

In the transfer matrix method, a cut-line bisecting the lattice is considered, which is moved to build conformations, cell by cell (Fig. 2). The main idea of the transfer matrix method is to count the number of partial conformations built up to the cut-line, and use this information to obtain the number of partial conformations when the cut-line is moved so that the next cell is incorporated into the lattice space for the partial conformation. This iterative procedure eventually leads to the full density of states when the cut-line reaches the top of the box and all the cells are incorporated. We will take the convention that the initial cut-line is at the bottom of the box, which is moved upwards as the algorithm proceeds. For a given row, the cells will be constructed from left to right. Denoting the coordinates of a cell as (i, j) $(1 \le i \le w,\ 1 \le j \le h)$, the cut-line has a kink on the right-hand side of the cell that is included in the partial conformation most recently, and consequently there are $w + 1$ edges in the cut-line (Fig. 2).

In an earlier version of the algorithm for SAW, the partially built conformations were classified according to their topology of the connection to the current cut-line [38]. In the improved newer version, they were classified by the connection topology of the part that is yet to be built, leading to a much simpler procedure for pruning out unnecessary conformations [37]. This topological information can be represented by a sequence of digits s_i $(i = 1, \ldots, w + 1)$, called the cut-line signature, associated with each edge of the cut-line. In the algorithm for SAW, each digit ranges from 0 to 3, where 0 represents no line crossing the edge, called the empty edge, 1 and 2 the left and the right stems of a loop, respectively, and 3 the free end [37]. The new element in the transfer matrix method for ISAW is that in order to keep track of the contact numbers of partial conformations, we need to introduce two types of empty edges depending on whether the site just below the empty edge is occupied or not, denoted by the digits 0 and 4, respectively. Therefore, in the algorithm for ISAW, each digit of the signature ranges from 0 to 4 (Fig. 2). We will refer to the edge with the digit 4 as being "charged". At most two digits of the signature can take the value 3, and the number of digits with the values 1 and 2 must be equal [37,38].

The number of partial conformations $F(n, k, v, s)$, called the partial density of states, is recorded for given values of the chain length