Parallel Algorithm for Calculation of the Exact Partition Function of a Lattice Polymer

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Abstract

We develop a parallel algorithm that calculates the exact partition function of a lattice polymer, by enumerating the number of conformations for each energy level. An efficient parallelization of the calculation is achieved by classifying the conformations according to the shape of the box spanned by a conformation, and enumerating only those in a given box at a time. The calculation time for each box is reduced by preventing the conformations related by symmetries from being generated more than once. The algorithm is applied to study the collapse transition of a lattice homopolymer on a square lattice, by calculating the specific heat for chain lengths up to 36.

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I. INTRODUCTION

Polymers on discrete lattices serve as a simple toy model of a polymer [1–6]. By introducing hydrophobic inter-monomer interaction, the lattice model can be used to study the collapse transition of a polymer [7–26]. Various quantities such as radius of gyration, end-to-end distance, and specific heat have been calculated, both using Monte Carlo samplings [8, 11, 16–22, 24–26] and exact enumeration [9, 12, 14, 23]. Although the length of chain that can be studied using exact enumeration is much less than that of the Monte Carlo sampling methods, the exactness of the calculation enables one to use powerful extrapolation methods to study the behavior of the lattice polymers in the limit of infinite chain length.

In the current study, we develop a method for calculating the exact partition function of a lattice polymer. The partition function is the most basic quantity from which all the important thermodynamic properties can be calculated. The number of states for each energy E, $\Omega(E)$, contains all the information needed for the calculation of the partition function Z, which is given by

$$Z(\beta) = \sum_E \Omega(E) e^{-\beta E}, \tag{1}$$

where $\beta \equiv 1/k_B T$ with the Boltzmann constant k_B and temperature T. In particular, it can be used for studying the collapse phase transition of the lattice polymer by observing behaviors of various quantities such as the specific heat,

$$C(T, N) = \frac{\partial E}{\partial T} = \beta^2 \frac{\partial^2 \ln Z}{\partial \beta^2}, \tag{2}$$

with increasing N.

Since the number of conformations is finite in the case of a lattice polymer, the partition function can be made a polynomial in $e^{-\beta}$ by considering models with integer values of E. To elaborate, we consider a polymer on regular lattice such as two-dimensional square or three-dimensional cubic lattices. Then the Hamiltonian for a heteropolymer is given by

$$\mathcal{H} = -\sum_{i<j} \epsilon(a_i, a_j) \Delta(\mathbf{r}_i, \mathbf{r}_j), \tag{3}$$

where

$$\Delta(\mathbf{r}_i, \mathbf{r}_j) = \begin{cases} 1 \ \ (|i-j| > 1 \quad \text{and} \quad |\mathbf{r}_i - \mathbf{r}_j| = 1) \\ 0 \ \ (\text{otherwise}), \end{cases} \tag{4}$$

a_i is the type of the i-th monomer, and $\epsilon(a,b)$ is the interaction energy between the monomers of type a and b. By taking $\epsilon(a,b)$ to be integer multiples of a unit energy ϵ, $\epsilon(a,b) = n(a,b)\epsilon$, the partition function is expressed as a polynomial:

$$Z = \sum_{\{\kappa(a,b)\}} \tilde{\Omega}(\{\kappa(a,b)\}) z^{\sum_{a,b} n(a,b)\kappa(a,b)} = \sum_K \Omega(K) z^K, \tag{5}$$

where $z \equiv \exp(\beta\epsilon)$, $\tilde{\Omega}(\{\kappa(a,b)\})$ is the number of polymer conformations with contact numbers $\{\kappa(a,b)\}$, and

$$\Omega(K) \equiv \sum_{\sum n(a,b)\kappa(a,b)=K} \tilde{\Omega}(\{\kappa(a,b)\}) \tag{6}$$

is the number of conformations with energy $E = -K\epsilon$. The homopolymer composed of only one kind of monomers is a special case where $n(a,b) = 1$ regardless of a, b, with K now being the number of intra-chain contacts.

In this work, we develop an efficient parallel algorithm for calculating the exact partition function of a lattice polymer by enumerating $\Omega(K)$. The parallelization is implemented by classifying the conformations by the shape of the box enclosing a conformation. Only the conformations corresponding to a given box is enumerated at a time by pruning partial conformations incompatible with the box, and the tasks of enumerating the conformations for the boxes are distributed among computational nodes. Since no communications are required during the calculation, the computational speed scales well with the number of CPUs. The calculation time for each box is reduced by exploiting the symmetries of the system. A conformation, its rotations by multiples of 90°, and their mirror images are considered equivalent and prevented from being generated more than once. For a generic conformation, the discrete rotations and reflections form an 8-fold and 48-fold symmetries in two and three dimensions, respectively. Exceptions are the cases of lower-dimensional conformations embedded in higher dimensional spaces. In two dimensions, a straight chain is the one-dimensional conformation, invariant with respect to reflection perpendicular to the chain, so the discrete rotations and reflections form a 4-fold symmetry. Similarly, in three dimensions, only 6-fold and 24-fold symmetries exist for the linear and planar conformations, since they are invariant under transformation perpendicular to the underlying plane and straight line.

Therefore, the number of conformations with discrete rotations and reflections considered distinct in D dimensions, $\Omega^{(D)}(K)$, can be easily obtained from the reduced number of

conformations $\tilde{\omega}^{(D)}(K)$ where symmetrically related conformations are counted only once and the lower-dimensional conformations are not counted:

$$\begin{aligned}
\Omega^{(1)}(K) &= 2\tilde{\omega}^{(1)}(K) = 2\delta_{K,0}, \\
\Omega^{(2)}(K) &= 8\tilde{\omega}^{(2)}(K) + 4\tilde{\omega}^{(1)}(K), \\
\Omega^{(3)}(K) &= 48\tilde{\omega}^{(3)}(K) + 24\tilde{\omega}^{(2)}(K) + 6\tilde{\omega}^{(1)}(K).
\end{aligned} \tag{7}$$

On the other hand, the reduced numbers of conformations $\omega^{(D)}(K)$ where only symmetries are eliminated, are expressed in terms of $\tilde{\omega}^{(D)}(K)$ as

$$\begin{aligned}
\omega^{(1)}(K) &= \tilde{\omega}^{(1)}(K) = \delta_{K,0}, \\
\omega^{(2)}(K) &= \tilde{\omega}^{(2)}(K) + \tilde{\omega}^{(1)}(K), \\
\omega^{(3)}(K) &= \tilde{\omega}^{(3)}(K) + \tilde{\omega}^{(2)}(K) + \tilde{\omega}^{(1)}(K).
\end{aligned} \tag{8}$$

From Eqs.(7) and (8), we see that $\Omega^{(D)}(K)$ are expressed in terms of $\omega^{(D)}(K)$ as:

$$\begin{aligned}
\Omega^{(2)}(K) &= 8\omega^{(2)}(K) - 4\delta_{K,0}, \\
\Omega^{(3)}(K) &= 48\omega^{(3)}(K) - 24\omega^{(2)}(K) - 18\delta_{K,0}.
\end{aligned} \tag{9}$$

It is to be noted that the enumeration in two dimensions must be performed before enumerating those in three dimensions.

Although the current algorithm may be used for both homopolymer and heteropolymer in any dimension, as a simple example of the application, we calculate the exact partition function for a homopolymer on a two-dimensional square lattice, for chain lengths up to 36. By analyzing the behavior of the specific heat, we could estimate the temperature of polymer collapse transition.

II. THE METHOD

The crucial ingredients in the current method are (1) classifying conformations according to the boxes they span, and enumerating only those for the given box at a time by pruning partial conformations incompatible with the box, and (2) preventing symmetrically related conformations from being generated more than once. The arguments are almost the same for both two and three dimensions, but more detailed illustration will be given for two dimensions which is easier to visualize.

A. The classification of the conformations according to the spanning boxes

For each conformation, we construct a rectangular box enclosing it, whose sides are touched. The conformations can then be classified according to the shapes of such boxes, since the box is uniquely determined for each conformation. The shape of a box can be described by the width w and height h in two dimensions, and the depth d is added for three dimensions. We use the convention that these numbers are measured in the unit of the lattice spacing, so the number of lattice sites spanned by the box is $(w+1)\cdot(h+1)\cdot(d+1)$. For simplicity of the discussion, we keep d regardless of the dimensions, which is 0 for two dimensions. As an illustration, conformations with box sizes 5×3 and 4×4 in two dimensions are depicted in Figure 1. There is an intrinsic direction in the polymer chain, and a conformation for N monomers can be considered as a self-avoiding walk of $N-1$ steps, starting from the 1st monomer.

Since the area or volume of a box should be large enough to accommodate a conformation, w, h, and d should satisfy the lower bound $(w+1)\cdot(h+1)\cdot(d+1) \geq N$ for a chain with N monomers. Also, since the perimeter of the box should be small enough so that all sides touch the conformation, they should also satisfy the upper bound $w+h+d \leq N-1$. Due to discrete symmetries, it is enough to consider only the boxes with $w \geq h \geq d$. Also, the conformations for boxes with w, h, and d that saturate the upper bound, $w+h+d = N-1$, do not have to be enumerated explicitly, since they can be obtained from a simple analytic formula. Considered as self-avoiding walks, these are the conformations where the steps are taken in a fixed direction along each axis, without turning back, making no intra-chain contact at all. Since there are D possible directions for each step in D dimensions, the total number of such conformations for all possible boxes is simply $D^{N-1}/D!$ when rotational and reflectional symmetries are eliminated. Therefore, the values of w, h, and d that have to be included in the explicit enumeration are integers bounded by the following inequalities:

$$\begin{gathered} w \geq h \geq d \\ (w+1)\times(h+1)\times(d+1) \geq N \\ w+h+d < N-1 \end{gathered} \tag{10}$$

where again d is set to 0 in two dimensions. The region of w and h where explicit enumeration is performed is shown in Figure 2 for the two-dimensional homopolymer along with the boundaries.

Only the conformations for a given box are enumerated at a time, and parallel computation is performed by distributing the boxes to the computational nodes. Since the number of boxes $N_{\rm box}$ is generally larger than the number of computational nodes $N_{\rm CPU}$, the simplest method of distribution would be to assign the same number of boxes to each node. However, this method turns out not to be so efficient since certain nodes finish jobs earlier and become free while others keep enumerating, due to the fact that the number of conformations and the computation time vary widely among the boxes. Therefore, the most efficient way of job distribution is to make enumeration for each box a separate task that can be taken up by any free node. Since a computational node that finishes the enumeration takes over a job in the queue, there is no idle time for any of the nodes. The total number of boxes for each chain length must be precalculated in order for this efficient distribution, which can be performed in a practically negligible amount of time. Absolutely no communication is needed between the nodes during the enumeration, and it is only after all the computations are finished that the results from all the nodes are added to obtain $\Omega(K)$. The current algorithm can be used in a single CPU as well, by requiring it to enumerate conformations for all possible boxes.

B. Self-avoiding walk and pruning

The conformations are enumerated by generating self-avoiding walks. This is most easily achieved by recursively calling a subroutine that makes one step into a given direction [27]. The number of sites n occupied by the current partial conformation is kept as a global variable, which is equivalent to the number of lattice sites visited by the walk so far. From the given position, the next step is made for each of the neighboring lattice sites not occupied by a monomer. For each step of the walk, the current lattice site is marked as occupied, and the contribution of the current monomer is added to the number of contacts K. When n reaches N, the contribution of the final monomer is added to K and $\omega(K)$ is incremented by one.

In order to ensure that the computation time is spent only for enumerating the conformations spanning a given box, any partial conformation incompatible with the current box is pruned out at an early stage. This is done by keeping the record of whether each side of the box has already been touched by the walk generated so far. If there is a boundary

that has not been touched as yet, whose distance from the current position is l, then the next step in the opposite direction to this boundary is forbidden unless there are sufficient number of remaining monomers $N - n$. Assuming the untouched boundary is at $x = 0$ and the current position is at $x = l$ and the next step is in the positive x direction, at least 3 monomers are needed to make a U-turn and get back to $x = l$, and l monomers are needed to reach the boundary $x = 0$, leading to the inequality

$$l + 3 \leq N - n, \tag{11}$$

which should hold for any step in the opposite direction from the untouched boundary, whose distance from the current position is l. Similarly, the next step in the direction orthogonal to the untouched boundary is forbidden unless

$$l + 1 \leq N - n. \tag{12}$$

C. Elimination of discrete symmetries

The speed of enumeration is increased by generating symmetrically related conformations only once. Since the discrete symmetries of rotation and reflection are 8-fold and 48-fold in two and three dimensions respectively, the enumeration time is reduced by nearly the same factor by calculating the reduced number of conformations $\omega(K)$ instead of the full number $\Omega(K)$. For a rectangular box where w, h, and d are all different, 90° rotational symmetry is removed by considering only the box with $w > h > d$. In order to remove the remaining 4-(8-)fold symmetry in two (three) dimensions, we divide the rectangular box into 4 (8) equivalent quadrants (octants) containing each corner of the box, and consider only the chain that starts inside one quadrant (octant), given by:

$$\begin{aligned} 1 \leq x \leq \tfrac{w}{2} + 1 \\ 1 \leq y \leq \tfrac{h}{2} + 1 \\ 1 \leq z \leq \tfrac{d}{2} + 1, \end{aligned} \tag{13}$$

where x, y, and z are integer coordinates for the lattice sites. The quadrant described by Eq. (13) in the case of two-dimensions is shown as gray area in Figure 3(a). Since symmetries are not completely eliminated for conformations starting at the boundaries, where any of the conditions, Eq. (13), is satisfied as an equality, additional constraints are imposed, so

that the first step along the axis corresponding to an equality is in the positive direction. For example, when w is an even number and if the starting position of the chain is at $x = \frac{w}{2} + 1$, we require that the first step along the x-axis should be positive. Examples in two dimensions are shown in Figures 3(b) and (c).

When any two of the three numbers w, h, and d are equal, for example $w = h$, there remains a reflection symmetry with respect to plane $x = y$, which is eliminated by imposing an additional constraint that among the steps parallel to the x-y plane, the first one must be along the x direction. Similarly, when $h = d$ we break the symmetry by requiring that among the steps parallel to the y-z plane, the first step must be along the y axis. Again the two-dimensional example is given in the Figure 3(d).

III. RESULT

The method developed in the current work can be applied to either heteropolymer or homopolymer in any dimension, but as a simple example of the application, we study the homopolymer in the two-dimensional square lattice. Since a monomer cannot make a contact with itself, as well as the nearest and next-nearest neighbors along the chain, the upper limit of the K summation in Eq. (5), denoted as $K_{\max}$, satisfies the upper bound

$$K_{\max} \leq \frac{N(N-5)n_{\max}}{2}, \tag{14}$$

where $n_{\max}$ is the maximum value of $n(a, b)$. In the absence of an additional information, we may take this value as the size of the array to store the values of $\omega(K)$, but for the special case of the homopolymer in two dimensions, we have the exact formula for $K_{\max}$ [28]:

$$K_{\max} = \begin{cases} N - 2m & \text{for } \; m^2 < N \leq m(m+1), \\ N - 2m - 1 & \text{for } \; m(m+1) < N \leq (m+1)^2, \end{cases} \tag{15}$$

where m is a positive integer.

We calculated the number of states $\omega(K)$ for $N \leq 36$. The same quantities for $N \leq 28$ have been calculated in earlier works [1, 28, 29]. Our calculation reproduce these results in the appropriate ranges. The new results for $29 \leq N \leq 36$ are presented in Table I and II. The CPU time using Intel Xeon CPUs (2.8GHz) is plotted in logarithmic scale as the function of N in Figure 4, for $15 \leq N \leq 30$ where time data are available. As expected, the

CPU time grows exponentially as N increases.

$$t \simeq A\lambda^N \tag{16}$$

where values of $A = 1.64(2) \times 10^{-8}$ and $\lambda = 2.43(2)$ are obtained by taking the log of Eq. (16) and performing the least square fit. The total number of conformations as well as the computational times of many enumeration algorithms are known to grow exponentially as μ^N where $\mu = 2.638$ is the connective constant for the self-avoiding walks [30], so the computational time of the current algorithm grows at somewhat slower rate than this. Although algorithms for enumerating the *total* number of conformations have been developed [31, 32] whose computation time grows at rates slower than the current one, it must be noted that the current method not only calculates the total number but also the number of conformations for each energy value, leading the calculation of the exact partition function at arbitrary temperature.

By the efficient distribution of the enumeration tasks among the computational nodes, the computational speed scales linearly with the number of computational nodes until the saturation occurs. It is obvious that the number of nodes used, $N_{\rm CPU}$, cannot exceed the number of boxes, but the saturation occurs at a smaller value of $N_{\rm CPU}$ because the enumeration time varies widely among the boxes. A few nodes enumerating the box with large number of conformations tend to keep computing even after most of the nodes have completed computations, causing the deviation from the linear scaling of computation speed with $N_{\rm CPU}$. By recording the computation times for each boxes and assuming the most efficient distribution of tasks between the nodes, the computation time could be calculated as a function of $N_{\rm CPU}$. The speed of computation, the inverse of the computation time, is plotted in Figure 5 for various values of N, where the saturated value of the speed is normalized to one. We see that the linear scaling holds for up to $N_{\rm CPU} = N_{\rm CPU}^{(\max)}$ which increases with N.

As an example of the application of our method, we calculate the specific heat per monomer,

$$C(T,N)/\epsilon^2 N = \frac{1}{\epsilon^2 N}\frac{\partial E}{\partial T} = \frac{\beta^2}{\epsilon^2 N}\frac{\partial^2 \ln Z}{\partial \beta^2} = \frac{(\ln z)^2}{N}\left[\frac{\sum_k k^2\Omega(k)z^k}{\sum_p \Omega(p)z^p} - \left(\frac{\sum_k k\Omega(k)z^k}{\sum_p \Omega(p)z^p}\right)^2\right] \tag{17}$$

which is plotted in Figure 6 as a function of z for several values of N. The finite N

approximation of the transition point, $z_c(N)$, is obtained from the condition $\frac{\partial C}{\partial z} = 0$. We observe a peak around $z \simeq 2$, which becomes sharper as N increases. The point of the collapse transition is known to follow the finite-size scaling

$$z_c(N) - z_c(\infty) \sim N^{-\phi}, \tag{18}$$

where ϕ is the crossover exponent whose exact value is believed to be 3/7 [15]. We apply the Bulirsch-Stoer extrapolation [33–35] to Eq. (18) and then obtain $z_c(\infty) = 2.07(7)$, equivalent to $T_c/\epsilon = 1.37(7)$, where the data for even N with $20 \leq N \leq 36$ were used. $z_c(N)$ is displayed in Figure 7 as the functions of $1/N$, along with the extrapolated value $z_c(\infty)$. The current result is in reasonable agreement with those from the earlier works.

IV. DISCUSSION

We developed an efficient parallel algorithm for calculating the exact partition function of a lattice polymer. An efficient parallelization of the calculation was achieved by classifying the conformations according to the shape of the box spanned by a conformation. Only the conformations corresponding to a given box were enumerated at a time, pruning partial conformations incompatible with the box at an early stage. The calculation time was further reduced by preventing the conformations related by symmetries from being generated more than once. The parallel efficiency could be maximized by requiring that any node that finishes the task of enumeration for a box takes over a new task of enumeration for another box whose conformations have not been enumerated by any of the nodes. As an illustration of applications, we studied the collapse transition of lattice homopolymers in square lattices, by calculating the specific heat. The exact partition function can also be used for calculating the partition function zeros in the complex temperature plane, which is a more sensitive indicator of the phase transition than the specific heat [36].

As mentioned in the previous section, the linear scaling of the computation speed with the number of CPUs $N_{\rm CPU}$ breaks down well before $N_{\rm CPU}$ reaches the total number of boxes, due to the fact the computation time varies wildly depending on boxes. However, considering the fact that $N_{\rm CPU}$ cannot be made arbitrarily large in practice, the saturation effect can be neglected in many situations, particularly when long chains are studied, since the saturation limit $N_{\rm CPU}^{(\rm max)}$ grows with the chain length N (See the Result). As can be seen from the

Result (See Fig.5), the partition function of the two-dimensional polymer chain of length 29 can be enumerated with up to 30 CPUs without saturation of the linear scaling, and one can employ more CPUs for studying chains of longer lengths. Since linear scaling becomes better as the chain length increases, our method is a powerful tool for studying long polymer chains with limited computational resources.

An idea of classifying conformations of two-dimensional homopolymers according to spanning boxes, similar to ours in certain aspects, has been introduced for the calculation of the partition function of a polymer on the square lattice at infinite temperature using transfer matrix formalism [32]. At least for such a calculation the transfer matrix was claimed to be superior to the direct counting, and it would be interesting to see whether it can be generalized for calculating the partition function at arbitrary temperatures in two dimensions, without introducing much additional computational costs. The current algorithm is more general in that not only the partition function at arbitrary temperature can be calculated, but heteropolymers and arbitrary dimensions can be treated in a straightforward manner. The explicit applications of the algorithm to these cases are left for future works.

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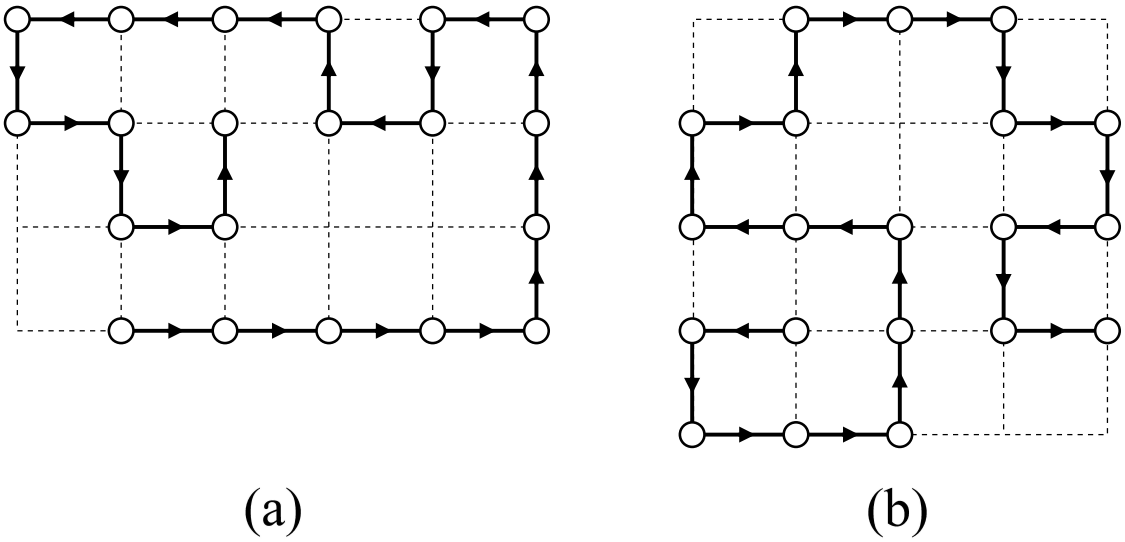

FIG. 1: Sample conformations for $N = 20$ on (a) 5×3 rectangle and (b) 4×4 rectangles. Circles are monomers of a lattice polymer and the arrow indicates the direction of the chain.

TABLE I: The number of conformations $\omega(K)$ on a square lattice as a function of the chain length $29 \leq N \leq 32$ and the number of contacts K.

K \ N	29	30	31	32
0	7689321701	17982126658	42108189098	98421806691
1	23540565448	56977682194	137862646874	332762640146
2	40085909835	100142920787	249700259569	620847470396
3	49071555164	126359874347	324279253784	829487165382
4	48771398860	129152420800	340420363856	894055572891
5	41585979484	113114869570	305828397226	823666234004
6	31508871807	87958369563	243684809928	672408321619
7	21617211324	61936948230	175770392578	496787988274
8	13642191086	40119932593	116592999110	337522862616
9	7980014626	24122755170	71817661842	213018321049
10	4362872816	13562820674	41372702687	125886832996
11	2226147024	7152132929	22391023650	69957624306
12	1065063681	3542639525	11397385748	36690896460
13	475157642	1646914139	5456762684	18158394435
14	194929001	716011778	2455124926	8476869526
15	72870960	286636733	1024918738	3722404274
16	24595083	104686477	393687071	1519486734
17	6751332	34676719	136943328	571834936
18	899613	9090306	41715633	194513054
19	16294	1005977	8866818	57891860
20		13498	636771	11290845
21				656376
Total	293922322781	784924528667	2092744741919	5584227078870

TABLE II: The number of conformations $\omega(K)$ on a square lattice as a function of the chain length $33 \leq N \leq 36$ and the number of contacts K.

K \ N	33	34	35	36
0	230322480773	538091763166	1258493243324	2938908879305
1	802996241232	1933501499531	4654740470620	11183769131112
2	1541179904025	3815982548374	9435546145403	23276263902178
3	2115681496986	5380293120526	13648570547310	34530182956163
4	2338726472743	6097828689993	15844205741060	41046002582789
5	2206962182754	5892600481193	15663662724418	41502969876897
6	1843564131938	5035936926127	13681123644389	37041494009397
7	1393031891232	3891460627050	10798327608646	29859153057072
8	967612822630	2763594584708	7829412575160	22103175375035
9	624333988838	1823442056984	5273396514658	15198342307484
10	377300221611	1127227716216	3327749067600	9793121298664
11	214525075976	656411900406	1978790499320	5948956055099
12	115237903606	361505461087	1113409518803	3422967752173
13	58512766632	188687694809	594317169744	1870659345753
14	28078596777	93399109108	301280956584	972915151671
15	12713385376	43768480489	144908527014	481649031145
16	5394346351	19397612212	66030540012	226685149424
17	2118111650	8050408136	28387608698	101251448207
18	763529938	3106194291	11380453744	42658656267
19	244420464	1095275398	4222218392	16800266331
20	64896504	342819455	1417505104	6127509709
21	9564594	87997218	412844504	2004417664
22	306498	11551406	89824129	573845730
23		265502	8277188	118501239
24			105265	9156136
25				57337
Total	14879374739128	39675824783385	105659884331089	281566759719981

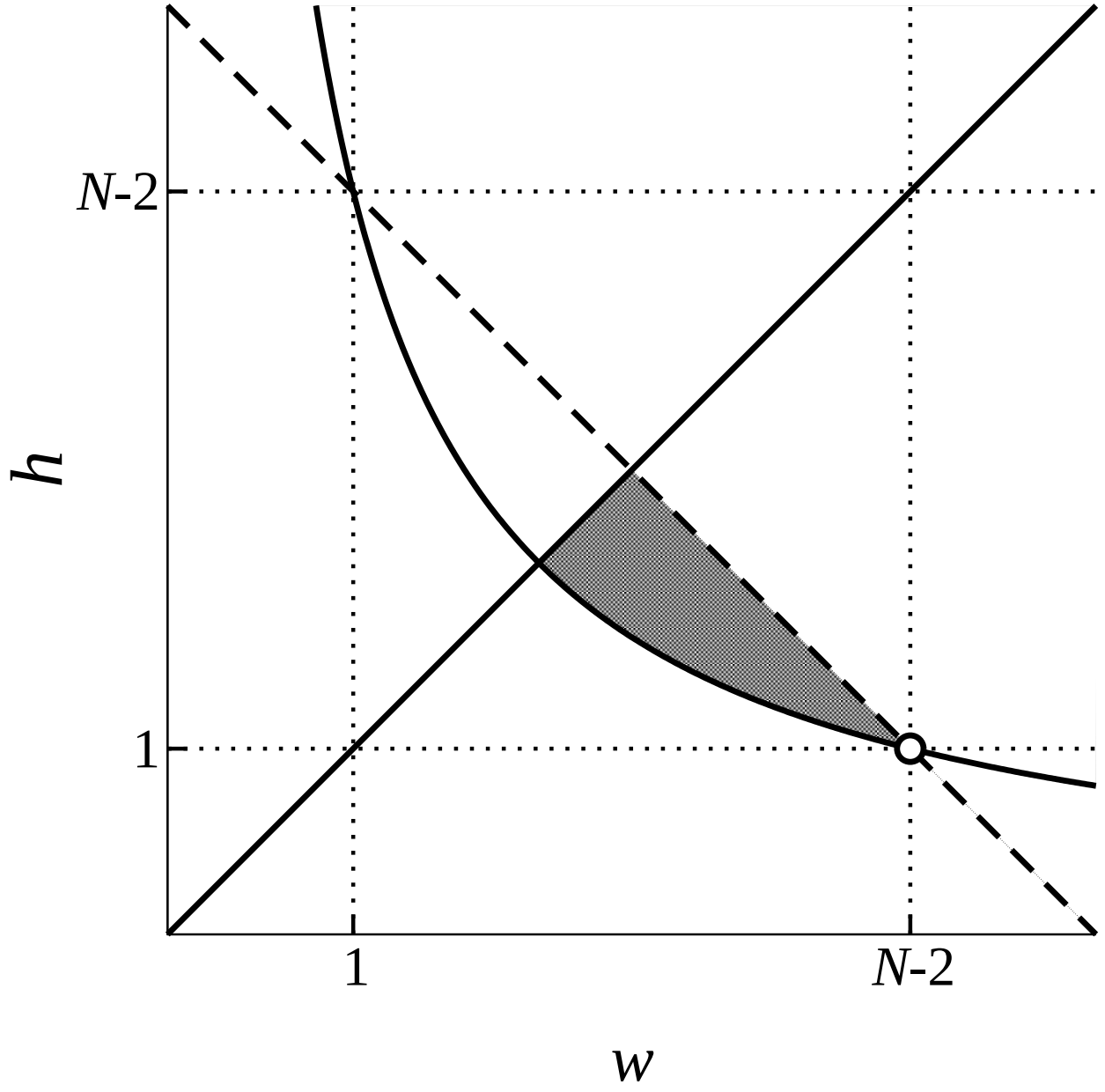

FIG. 2: The values of the box width w and height h for which the explicit computations are performed in two dimensions, are the points with integer coordinates inside the shaded area. The dashed line and the intersection point denoted by the white circle is not included (see text).

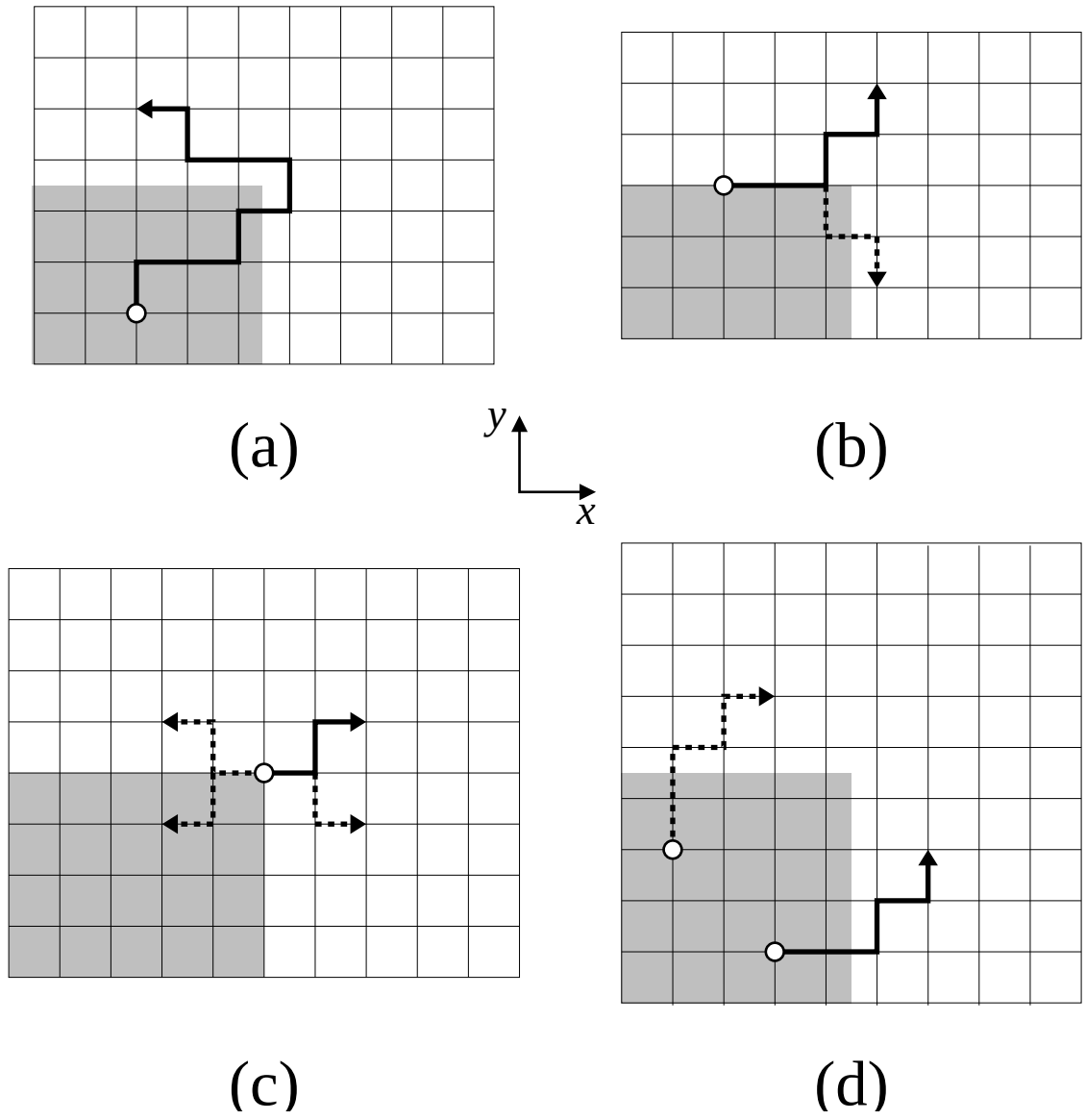

FIG. 3: (a) Because of the symmetries, only chains starting from the sites in a shaded area at the lower left corner are considered. (b) In the special case of chains starting at the boundary line $y = \frac{h}{2} + 1$, an additional constraint is imposed so that the first vertical step is in the upper direction. A similar constraint is imposed for a chain that starts at the boundaries $x = \frac{w}{2} + 1$ so that the first horizontal step is in the right direction. (c) For a chain starting at the center point with $x = \frac{w}{2} + 1$ and $y = \frac{h}{2} + 1$ the two constraints for the horizontal and vertical boundary are imposed simultaneously. (d) For a square box, the additional reflectional symmetry with respect to the line $y = x$ is eliminated by requiring that the first step is in the horizontal direction.

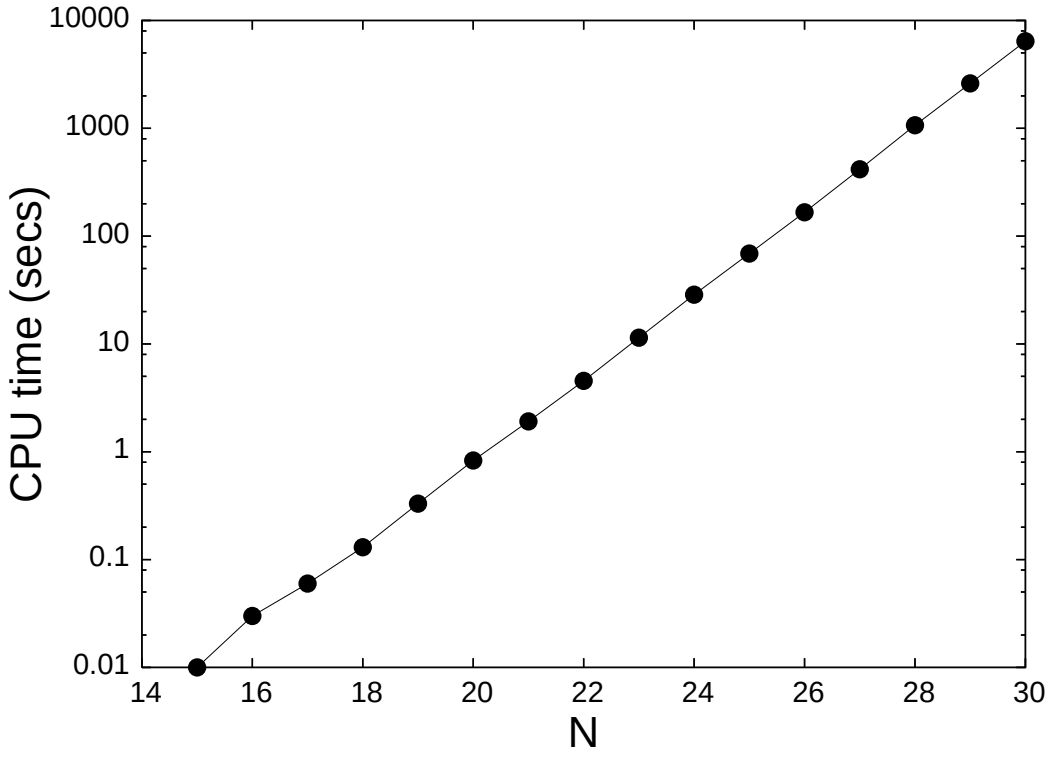

FIG. 4: The CPU time in log scales, plotted as a function of the chain length N.

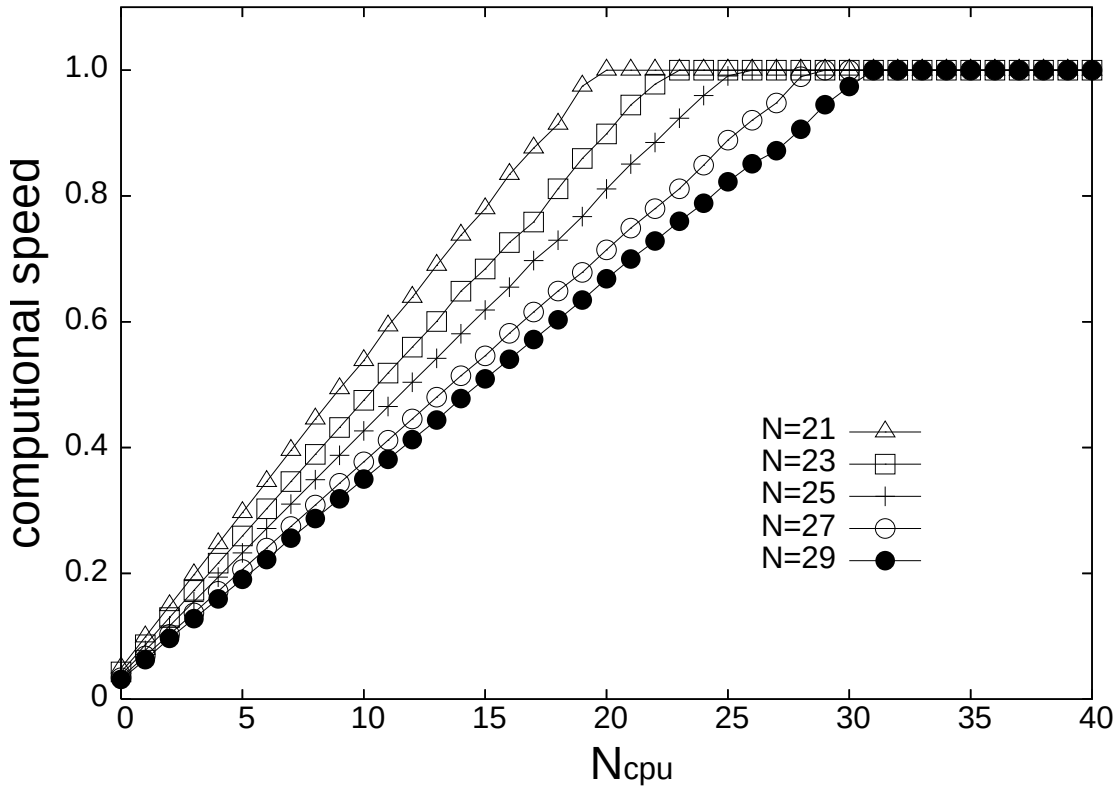

FIG. 5: The computational speed as the function of the number of computational nodes. The computational speed is defined as the inverse computational time, normalized so that its saturated value is 1.00.

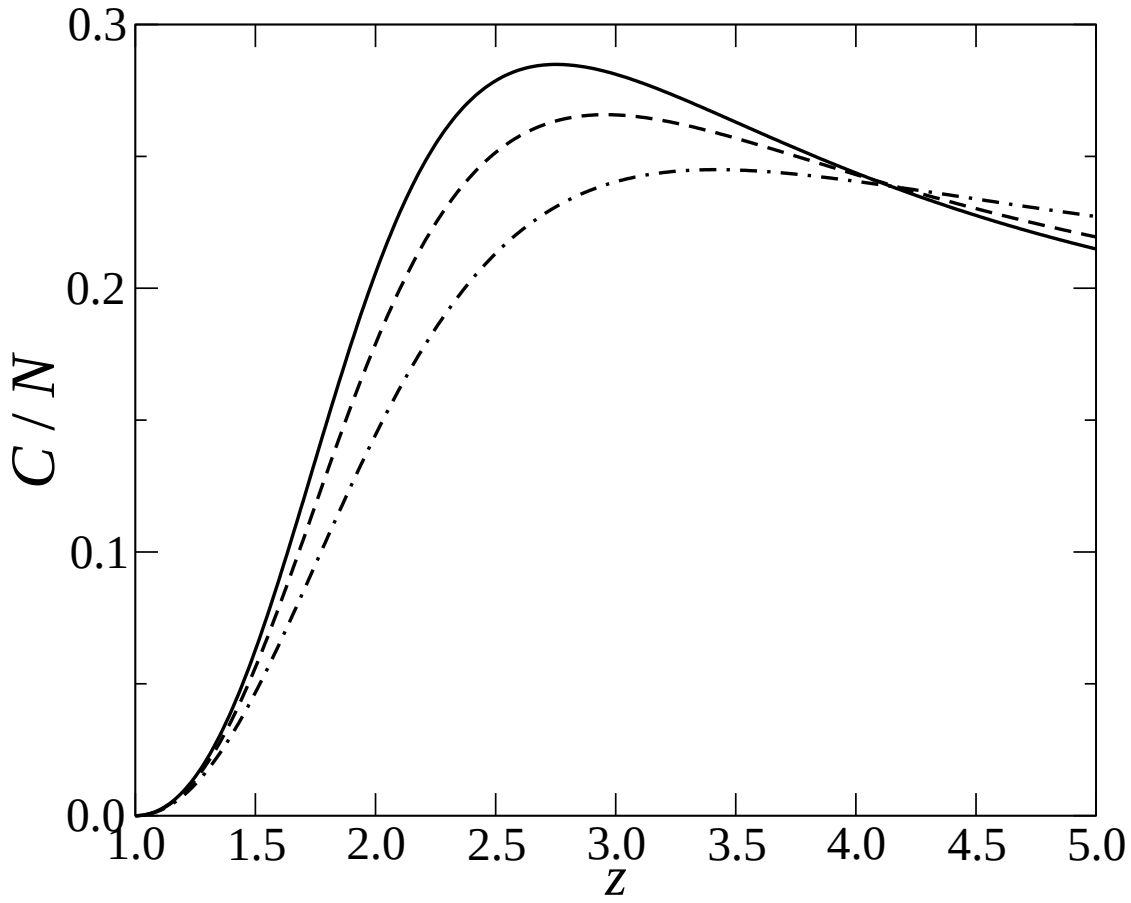

FIG. 6: The specific heat for $N = 20$, 28, and 36 from bottom to top.

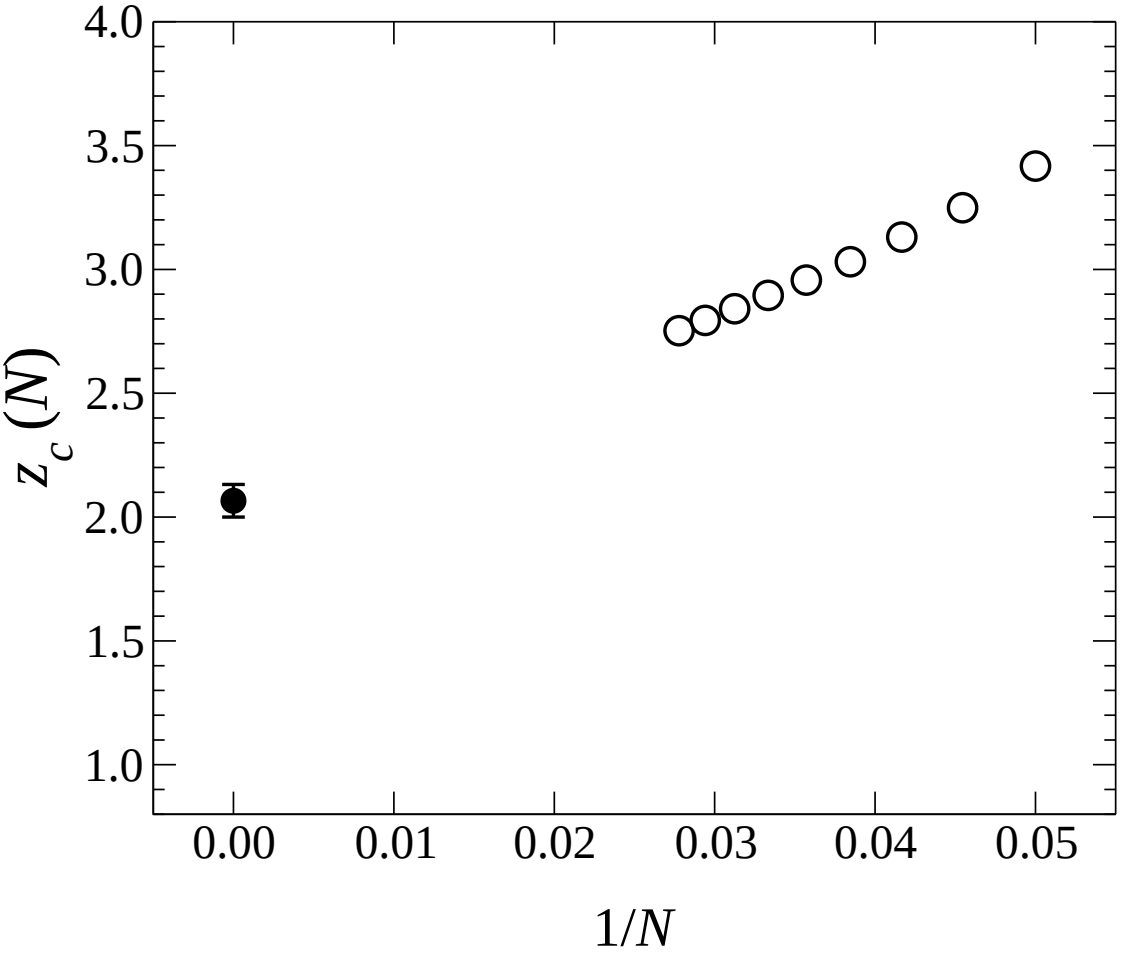

FIG. 7: The finite value approximation of the transition point z_c and its extrapolated value at $N = \infty$.