Exact enumeration of Hamiltonian circuits, walks and chains in two and three dimensions

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Abstract
We present an algorithm for enumerating exactly the number of Hamiltonian chains on regular lattices in low dimensions. By definition, these are sets of $k$ disjoint paths whose union visits each lattice vertex exactly once. The well-known Hamiltonian circuits and walks appear as the special cases $k = 0$ and $k = 1$, respectively. In two dimensions, we enumerate chains on $L \times L$ square lattices up to $L = 12$, walks up to $L = 17$ and circuits up to $L = 20$. Some results for three dimensions are also given. Using our data we extract several quantities of physical interest.

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1. Introduction

The subject of Hamiltonian circuits and walks plays an important role in mathematics and physics alike. Given a connected undirected graph $G$, a Hamiltonian circuit (or cycle) is a cycle (i.e., a closed loop) through $G$ that visits each of the $V$ vertices of $G$ exactly once. In particular, a Hamiltonian circuit has length $V$. Similarly, a Hamiltonian walk (or path) is an open non-empty path (i.e., with two distinct extremities) of length $V - 1$ that visits each vertex exactly once. Note that a Hamiltonian circuit can be turned into a Hamiltonian walk by removing any one of its edges, whereas a Hamiltonian walk can be extended into a Hamiltonian circuit only if its end points are adjacent in $G$.

We add now to this list of well-known definitions the set $C_k$ of Hamiltonian chains of order $k$. Each member in $C_k$ is a set of $k$ disjoint paths whose union visits each vertex of $G$ exactly once (see figure 1). The set of Hamiltonian walks is then $C_1$, and by convention we shall let $C_0$ denote the set of Hamiltonian circuits. Note that if $V$ is even, $C_{V/2}$ is the set of

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1 This name is in honour of the Irish mathematician W R Hamilton, who in 1857 developed a game whose object (in mathematical terms) is to find a Hamiltonian circuit on a planar projection of the dodecahedron. See http://puzzlemuseum.com/month/picm02/200207/icosian.htm.
dimer coverings of $G$. The Hamiltonian chain problem has been studied earlier by Duplantier and David on the Manhattan lattice [1], but never to our knowledge on an undirected lattice.

Determining whether $G$ contains a Hamiltonian circuit is a difficult (NP-complete) problem. An even more difficult problem is to determine how many distinct Hamiltonian circuits are contained in $G$. In this paper, we shall present an algorithm that efficiently enumerates Hamiltonian circuits, walks and chains for regular low-dimensional graphs.

The motivation for studying such Hamiltonian structures is by no means limited to graph theory. Indeed, under appropriate solvent conditions, biopolymers such as proteins may fold to form compact conformations, the study of which is currently at the centre of an intense activity in the biophysics community. While real biopolymers contain complicated interactions which can probably not be fully accounted for within any simple lattice model, the study of Hamiltonian walks has been advocated as a first approximation for understanding qualitatively the excluded-volume mechanisms at work behind such problems as polymer melting [2] and protein folding [3]. Our extension to Hamiltonian chains permits us to study polydisperse models of several polymers.

Another interest stems from the study of magnetic systems with $O(n)$ symmetry in physics. These can be modelled on the lattice as self-avoiding loops (each having the weight $n$) [4], which, in the limit of vanishing temperature $T$, are constrained to visit all the vertices [5]. Coupling such systems to a magnetic field $H$ amounts, in a perturbative expansion around $H = 0$, to inserting pairs of loop end points [6]. In the limit $n \to 0$, the partition function $Z$ of the $O(n)$ model at $T = 0$ in a weak magnetic field $H$ can thus be expressed in terms of the number of Hamiltonian chains as

$$Z = \sum_k C_k H^{2k}.$$  \hfill (1.1)

Finally, the exact enumeration of configurations is useful for settling issues of ergodicity when developing algorithms that provide unbiased sampling of Hamiltonian walks in two [7] and three [8] dimensions.

In section 2, we present our enumeration algorithm and discuss some aspects of its implementation. Results in dimensions $d = 2$ and $d = 3$ are given in section 3. For convenience, we limit the discussion to the simplest lattices (square and cubic), although the construction extends straightforwardly to any regular lattice. Our results are strongest in $d = 2$ where we determine all $C_k$ for $L \times L$ square lattices up to $L = 12, C_1$ up to $L = 17$ and $C_0$ up to $L = 20$. In $d = 3$, the largest lattice that we were able to access has size $3 \times 4 \times 4$. Finally, we show in section 4 how to extract physically interesting quantities from our data.
2. Algorithm

We first present our algorithm in dimension $d = 2$ and then discuss the necessary modifications for $d = 3$. For convenience, we limit the presentation to the simplest lattices, namely an $L_1 \times L_2$ square lattice and an $L_1 \times L_2 \times L_3$ cubic lattice, although the construction extends straightforwardly to any regular lattice. The boundary conditions are free (non-periodic), although it will be clear that it is easy to introduce periodic boundary conditions along one of the lattice directions.

The algorithm is based on the transfer matrix principle, according to which the lattice is cut into two parts by means of a conveniently chosen $(d - 1)$-dimensional oriented surface $S$. The part of the lattice above (resp. below) $S$ is called the future (resp. the past). The surface $S$ cuts the lattice only at mid points of edges.

At the initial (resp. final) step of the enumeration the whole lattice belongs to the future (resp. past), so the algorithm consists in sweeping $S$ over the entire lattice. This is done by gradually pushing $S$ towards the future, so that in any one step of the algorithm a single vertex is transferred from the future to the past. A few subsequent steps for a $4 \times 4$ lattice are shown in figure 2.

In any step, the configuration of the system is described by some information about the edges cut by $S$ and by the number $k$ of chains which have already been completed. The information referred to is the connectivity of the cut edges with respect to the part of the lattice which belongs to the past, and is best illustrated by an example (see figure 3). The complete description of the configuration reads in this case $(0, 1, 1, 2, 3, 2|0|1)$, where the first $L_1$ entries refer to the state of the cut edges which are parallel to the 2-direction (vertical), and the next entry refers to the state of the one cut edge which is parallel to the 1-direction (horizontal). The last entry is the number $k = 1$ of completed chains. In the connectivity part of the information, we use the following coding:
(i) A zero entry means an empty edge.

(ii) Two equal positive entries mean a pair of edges which are connected in the past by part
of a chain. Each of these edges will eventually have to be linked to a chain end point in
the future, so as to form a complete chain.

(iii) An unpaired positive entry means an edge which forms part of a partially completed chain,
one end point of which has already been fixed in the past. The edge will eventually be
linked to another end point in the future, leading to the formation of a complete chain.

It is important to avoid any redundancy in this connectivity information. A unique coding
is obtained by requiring that the positive entries (i.e., unpaired entries, or the leftmost member
of a pair of equal entries) be arranged in increasing order \((1, 2, 3, \ldots)\) when reading through
the coding from left to right.

In step \(t\) of the enumeration, the configurations are transferred from `time’ \(t\) to time
\(t + 1\). More precisely, each configuration at time \(t\) is examined in turn, and all its descendent
configurations at time \(t + 1\) are generated by exhausting the possible arrangements of the chain
at the vertex which is transferred from the future to the past. The information described above
is necessary and sufficient for deducing the connectivity information at time \(t + 1\) from that
at time \(t\). Note that since the transferred vertex is not allowed to be empty, there are four
possible arrangements if it accommodates a chain end, and six arrangements if a chain passes
though it.

Each configuration generated at time \(t + 1\) is inserted in an appropriate data structure—a
hash table— which also keeps track of its weight (here an integer). The weight of a descendent
configuration is the sum of the weights of all the parent configurations that generated it. Some
of the generated descendent configurations are however 
\textit{rejected} before insertion in the hash
table (see below). Once step \(t\) has been completed, the hash table storing the configurations at
time \(t\) is erased, and one can move on to step \(t + 1\). In this way, only two hash tables (at times
\(t\) and \(t + 1\)) are needed in the entire process.

Note that the choice of data structure is essential for the feasibility and the efficiency of
the algorithm. A hash table permits us to store the configurations via a key which is obtained
by reading its coding as one large integer, modulo a suitably chosen prime. Storing and
retrieving configurations can be done in constant time, i.e., independently of the number of
configurations being stored in the hash table.

The hash table also allows us to keep track of the weight of each configuration, according
to the above rule. Namely, when a descendent configuration is generated with weight \(w\), we
first make an attempt of looking it up in the hash table at time \(t + 1\). If it is not there, it is
inserted with weight \(w\). If it is already there, \(w\) is added to the weight of configuration already
present.

If in the transfer process the two ends of the same chain (coded by two equal positive
entries) join up, the resulting configuration is rejected, since this would mean forming a cycle
rather than a chain. (We make an exception to this rule when the very last vertex is added,
since this permits us to enumerate \(C_k\).) If an unpaired positive entry gets left behind in the past
it means that a chain has been completed, and so \(k \rightarrow k + 1\).

Denote now a general configuration as \((s_{2,1}, s_{2,2}, \ldots, s_{2,L_1}, |s_1|k)\). At step \(t = 0\), the
initial state is \((0, 0, \ldots, 0) |0|0\) and has weight 1. When a row of the lattice is completed, any
configuration with \(s_1 \neq 0\) gets rejected. When transferring the \(i\)th vertex of the last row, any
configuration with \(s_{2,i} \neq 0\) gets rejected. This trick allows us to avoid having to deal with
a lot of special cases when a boundary vertex is transferred—and also makes it much easier
in practice to implement the algorithm correctly. After step \(t = L_1L_2\) the lattice belongs
completely to the past, and all the configurations are of the form \((0, 0, \ldots, 0) |0|k\). Their
respective weights are precisely \(C_k\) that we wanted to compute.
The maximum lattice size that we can attain is essentially limited by the number of different intermediate configurations generated in the transfer process. This number attains its largest value after transferring the next last vertex in the next last row. In practice we could store at most \( \sim 10^9 \) configurations.

As usual in enumeration studies, the coefficients \( C_k \) are much larger than the integers which are usually represented by a computer (\( \leq 2^{32} \) for an unsigned integer on a 32 bit machine). We therefore repeat the enumeration several times, computing each time the result modulo different coprime integers \( (2^{32}, 2^{31} - 1, 2^{31} - 3, \ldots) \), and reconstruct the true result in the end by using the Chinese remainder theorem. Note that the use of modular arithmetics is possible because the weights of configurations are constructed only by successive additions of positive integers.

The counts for systems of size \( L_1 \times L_2 \) and \( L_2 \times L_1 \) should of course coincide. Verifying that this is indeed the case is however a very strong check of the algorithm, since permuting \( L_1 \) and \( L_2 \) (with \( L_1 \neq L_2 \)) leads to a completely different transfer process in terms of the propagation of the surface \( S \). We have performed such checks both for \( d = 2 \) and \( d = 3 \).

We now briefly describe how the algorithm can be adapted to a \( d \)-dimensional hypercubic lattice of size \( L_1 \times L_2 \times \cdots \times L_d \). The surface \( S \) is pushed though the lattice by means of \( d \) nested loops, of which the innermost loop (at nesting level \( d - 1 \)) moves \( S \) along the \( 1 \)-direction, etc, and the outermost loop (at nesting level 0) moves \( S \) along the \( d \)-direction. In general, the loop at nesting level \( \ell \) moves \( S \) along the \( (d - \ell) \)-direction.

A configuration is given by \( \{s_{d-1}\} \times \{s_{d-2}\} \times \cdots \times \{s_1\} \), where the space \( \{s_i\} \) describes the edges cut by \( S \) which are parallel to the \( \ell \)-direction and consists of \( \prod_{i=1}^{d-\ell} L_i \) entries. When the loop at nesting level \( d - \ell \) is executed for the last time, the entry in \( \{s_{\ell}\} \) corresponding to the position of the loops at nesting levels \( > d - \ell \) must be zero; otherwise the configuration is rejected.

At each vertex there are \( 2d \) possible local arrangements if the vertex contains a chain end, and \( \binom{2d}{2} \) arrangements if it does not.

We have implemented the algorithm for \( d = 2 \) and \( d = 3 \). It is of course most efficient in low dimensions where the number of entries necessary to describe a configuration is small, and the configurations themselves are strongly constrained by topology. We were however able to obtain useful results as well for \( d = 3 \) (see below).

### 3. Results

#### 3.1. Two dimensions

We first present our results in two dimensions.

We have been able to solve the full Hamiltonian chain problem for \( L \times L \) square lattices up to size \( L = 12 \). The number of circuits \( C_0 \) vanishes when \( L \) is odd by an easy parity argument, but the remaining \( C_k \) with \( k = 1, 2, \ldots, [L^2/2] \) are all non-zero. The complete result for \( L = 12 \) is shown in table 1.

When \( L \) is even, \( C_{L^2/2} \) should be the number \( D_L \) of dimer coverings of an \( L \times L \) square lattice. We have checked that our data agree with the analytical results [9] for \( D_L \) for all \( L = 2, 4, 6, 8, 10, 12 \).

If only the first few \( C_k \) are needed, the enumeration can be taken to larger sizes by rejecting all states \( \{s_{2,1}, s_{2,2}, \ldots, s_{2,d}, \{s_1\} \} \) with \( k > k_{\text{max}} \).

In particular, we have obtained the number \( C_1 \) of Hamiltonian walks up to size \( L = 17 \), see table 2. This extends the \( L \leq 7 \) results of Mayer et al [10] by ten new terms. Note also
Table 1. Number $C_k$ of Hamiltonian chains of order $k$ (i.e., consisting of precisely $k$ chains) on a $12 \times 12$ square lattice.

| $k$ | $C_k$ |
|-----|-------|
| 0   | 1076226888605605706 |
| 1   | 34526648593243754220 |
| 2   | 41050490909901274255863352 |
| 3   | 1716401559105997979087993260 |
| 4   | 363652056217129712602430353540 |
| 5   | 4614804195743592698824499692732 |
| 6   | 3870392655399660347471749180958852 |
| 7   | 2290044479738768805213214595470648 |
| 8   | 10014026193777241299766968086305774 |
| 9   | 33512632781634776435981605808153310160 |
| 10  | 88182988738744412162695871243309826506 |
| 11  | 1864253641509238433216389461927330172268 |
| 12  | 32225643570878494867009058887596660853042 |
| 13  | 4621682292162998143746281985324396507245748 |
| 14  | 5566937778738626082978946983863634701817981938 |
| 15  | 56907591266119765796588082616146969526622268 |
| 16  | 498128553355287563649851394837399217879495404 |
| 17  | 376259525355799790490876556302907957367971441020 |
| 18  | 2469068810121023544317004188530713590945411914 |
| 19  | 14192586038547811892361610528258465090872582482860 |
| 20  | 71328606843660293095526723817890226149324996051770 |
| 21  | 317097933444980244064203429296046128253752002853220 |
| 22  | 124908447120415462309161399602853755323216171859772 |
| 23  | 437544158500731873816634769735563649135514407725428 |
| 24  | 13673227330703731916940496493595296405766113534103766 |
| 25  | 382270415781777829399272623888324831630328689485072 |
| 26  | 9585454312915970883751499759209798436298141104060618 |
| 27  | 21605432415261909273142199238522975041539861478121508 |
| 28  | 438604274185012335575530043782600945755207568623643594 |
| 29  | 803320261178156379151403166347291125863198470203538048 |
| 30  | 13294136091618991378849781072357759426127805779481138 |
| 31  | 1990427307509569440202368471248086663998155541297504096 |
| 32  | 269911872613239697241170136925985393385382309591724116 |
| 33  | 331804099625224925481740087801704155429556174343699608 |
| 34  | 370035927341155923554786919768922871409843218081792948 |
| 35  | 37458754807609851743974309775047365033853657449987776 |

that Jaeckel et al [11] have proposed a Monte Carlo method for estimating $C_1$ for larger $L$. These authors obtain $1.3582 \times 10^7$ for $L = 7$—that is 0.3% above the exact result—and $2.7791 \times 10^9$ for $L = 8$—that is 29% below the exact result.

Varient Hamiltonian walks, constrained to have their end points on diametrically opposite corners of an $L \times L$ square have been studied for $L = 17$ in [13]. (For odd $L$ these walks were permitted to leave exactly one vertex of the lattice uncovered.) This is technically an easier problem than the unconstrained walks considered here.

Finally, we have obtained the number $C_0$ of Hamiltonian circuits up to size $L = 20$, see table 3. This extends the $L \leq 16$ data [13] by two new terms.
3.2. Three dimensions

Our results for the full Hamiltonian chain problem on small $L_1 \times L_2 \times L_3$ parallelepipeds are given in Table 4. In addition, we find for the $3 \times 4 \times 4$ system a number of $C_0 = 3777388236$ circuits and $C_1 = 1073054619800$ walks.

Note that the transfer matrix method is essentially limited by the area of the smallest cross section of the parallelepiped. It would thus be possible to extend the enumerations to some systems with, say, $L_1 = L_2 = 3$ and $L_3 \geq 5$, but we have chosen to focus here on close-to-cubic shapes which are the most challenging.

The number of walks $C_1$ has been much studied in the area of protein research [14, 15], whereas the numbers $C_k$ with $k \neq 1$ have to our knowledge not been considered previously. Note that the works [14, 15] were based on direct enumeration, meaning that in contrast to our

| $k$ | $C_k$ |
|-----|-------|
| 36  | 344370502558807229056235400083638573226282048855221139030 |
| 37  | 2875008789367922659848083522244722363355224468273444202 |
| 38  | 218049376147564520077617976768534387807056101785154 |
| 39  | 15020953917067157577298701307666462995527212507397512 |
| 40  | 93967724819776393885392911646530135042650207872340 |
| 41  | 53356285381548553419279650972101468170748332264456 |
| 42  | 2748624906969290252299091062079057175932329091824 |
| 43  | 12836255399747371943487735257952630895867479747624 |
| 44  | 542949685108651628368281323909718526262924214932 |
| 45  | 20778008123924341362785234236813392470106157931284728 |
| 46  | 71874688457846504253127092326201986740490532776292 |
| 47  | 2241482341086337068944007492030775581030693310936 |
| 48  | 62982381571595313333156488999194041468765091268042 |
| 49  | 159077245534404479333245529316240004384667375966020 |
| 50  | 36305273248074555220433523468060710122229094542106 |
| 51  | 73025439102881235299361943495060798679283726808 |
| 52  | 13200742150311062421248738659331692519827058055405664 |
| 53  | 21217240913663799011066295762956529242562898136 |
| 54  | 3029994014815631520746187262186209324083454 |
| 55  | 37946682495061005682688766663833536523653816 |
| 56  | 418512742391130986282686888840526291044063692 |
| 57  | 4031033142453656820268520958344353430213252 |
| 58  | 336925505474814797946214848424889586369652 |
| 59  | 242794327043218279242923744503680409745316 |
| 60  | 14951909347540990085112030789218715790 |
| 61  | 7794936474077163638082299007304562711536 |
| 62  | 3401268809654579976214776969372499928 |
| 63  | 12253433732360441191970933819722548 |
| 64  | 35847082989635138579598770248538788 |
| 65  | 83422315118501510474256627439696 |
| 66  | 1504401207221433196476714201368 |
| 67  | 2031231995130550246186136496 |
| 68  | 195891861059335966516705296 |
| 69  | 12602334728369293472453184 |
| 70  | 4853990585658564517760 |
| 71  | 9190437822899701504 |
| 72  | 5306047752196000 |

Table 1. (continued.)
Table 2. Number $C_1$ of Hamiltonian walks on an $L \times L$ square lattice, up to size $L = 17$.

| $L$ | $C_1$ |
|-----|-------|
| 2   | 4     |
| 3   | 20    |
| 4   | 276   |
| 5   | 4324  |
| 6   | 229348|
| 7   | 15355280 |
| 8   | 3023313284 |
| 9   | 745416341496 |
| 10  | 730044829512632 |
| 11  | 786671485270308848 |
| 12  | 3452664855804347354220 |
| 13  | 1665200571760534681315580 |
| 14  | 331809088406733654427925292528 |
| 15  | 7263611367960266490262600117251524 |
| 16  | 662634717384979793238814101377988786884 |
| 17  | 6642899473915946996440119579736807612665540 |

Table 3. Number $C_1$ of Hamiltonian circuits on an $L \times L$ square lattice, up to size $L = 20$.

| $L$ | $C_0$ |
|-----|-------|
| 2   | 1     |
| 4   | 6     |
| 6   | 4638576 |
| 8   | 467260456608 |
| 10  | 1076226888605665706 |
| 12  | 56126499620491437281263608 |
| 14  | 65882516522625836326159786165530572 |
| 16  | 173392637788896183927790794055670829347983946 |
| 18  | 102046042736076879354302696567512831571073052662428097106 |

The enumerations reported above contain many quantities of physical relevance. We discuss here some of them.
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Table 4. Number $C_k$ of Hamiltonian chains of order $k$ on various cubic lattices of size $L_1 \times L_2 \times L_3$. Blank entries are zero.

| $k$ | $2 \times 2 \times 2$ | $2 \times 2 \times 3$ | $2 \times 3 \times 3$ | $3 \times 3 \times 3$ | $3 \times 3 \times 4$ |
|-----|----------------------|----------------------|----------------------|----------------------|----------------------|
| 0   | 6                    | 22                   | 324                  | 0                    | 3918744              |
| 1   | 72                   | 584                  | 16880                | 2480304              | 677849536            |
| 2   | 204                  | 4204                 | 270756               | 104844792            | 40656040968          |
| 3   | 108                  | 7604                 | 1281376              | 1246834176           | 816646740296         |
| 4   | 9                    | 4541                 | 2507084              | 6520250088           | 7803954743412        |
| 5   | 852                  | 2281064              | 17852434656          | 41553510978656       |
| 6   | 32                   | 985354               | 27873228036          | 134709106959932      |
| 7   | 190580               | 25864316448          | 280608712776492      |
| 8   | 13834                | 14445212196          | 388267754276278      |
| 9   | 229                  | 4798350687           | 363680422635635      |
| 10  | 911288760            | 232420898624633      |
| 11  | 91325100             | 101132591631452      |
| 12  | 4119048              | 29594655770318       |
| 13  | 57048                | 5683316575620        |
| 14  | 687432832414         |
| 15  | 49991382300          |
| 16  | 1837669320           |
| 17  | 29304199            |
| 18  | 117805              |

Table 5. Probability $p_{\text{adj}}$ that the two end points of a Hamiltonian walk on an $L \times L$ square lattice are adjacent.

| $L$ | $p_{\text{adj}}$ |
|-----|------------------|
| 2   | 1.00000000000000000000 |
| 4   | 0.34782608695652173913 |
| 6   | 0.16826830842213579364 |
| 8   | 0.09819321919798768694 |
| 10  | 0.064004351201727304050 |
| 12  | 0.04488610346836087660 |
| 14  | 0.03315398616246303584 |
| 16  | 0.02545282308230371747 |

4.1. Conformational exponents

The radius of gyration $R$ of a polymer of length $l \gg 1$ is expected to scale like

$$R \sim l^{\nu}$$  \hspace{1cm} (4.1)

where $\nu$ is a standard critical exponent [6]. For Hamiltonian walks on an $L^d$ hypercube in $d$ dimensions, we have obviously $R \sim L$ and $l \sim L^d$, and so $\nu = 1/d$. Non-trivial information is however contained in the number of circuits and walks, here both supposed to have one marked monomer attached to a fixed point:

$$\tilde{C}_1 \sim \mu l^{\nu-1}, \quad \tilde{C}_0 \sim \mu l^{-\nu d}. \hspace{1cm} (4.2)$$

Here $\mu$ is the so-called connective constant and $\gamma$ is another critical exponent [6]. In our set-up, the circuits are unmarked and the end points of the walks are free to be anywhere on the lattice, and so

$$C_1/C_0 \sim l^{\nu+1} \sim L^{(\nu+1)d}. \hspace{1cm} (4.3)$$
In addition to this leading behaviour there are subdominant corrections due to surface effects.

In two dimensions, we can extract results for $\mu$ and $\gamma$ using the data in tables 2 and 3. Due to parity effects, this is best done by working in terms of the ratios $\eta(L) = C_0(L)$ for even $L$ or $C_1(L)$ for any parity in the case of $\mu$, and $\eta(L) = C_1(L)/C_0(L)$ for even $L$ in the case of $\gamma$. The naive approximants are further extrapolated using standard finite-size scaling techniques. This gives

$$\mu = 1.473 \pm 0.001, \quad \gamma = 1.042 \pm 0.003. \quad (4.4)$$

Our estimate for $\mu$ is in good agreement with (but less accurate than) the currently best-known estimate [5]

$$\mu = 1.472801 \pm 0.00001. \quad (4.5)$$

Note that the latter uses exact predictions from field theory for the leading finite-size corrections, a scheme that we have not adopted here. The constrained Hamiltonian walks considered in [12] led to a consistent value for $\mu$. The long-standing history of numerical and analytical estimates for $\mu$ of Hamiltonian walks can be found in the introductions of [5, 11].

Our estimate for $\gamma$ is a nice confirmation of the exact field theoretical result [5]

$$\gamma = \frac{117}{112} = 1.04464\ldots \quad (4.6)$$

Previous numerical results, as discussed in [5] and references therein, were obtained in a cylindric geometry and assumed certain results of conformal field theory. The present estimate therefore furnishes a more direct verification of the exact result (4.6).

4.2. Contact probabilities

As already mentioned in the introduction, a Hamiltonian circuit can be turned into a Hamiltonian walk by removing any one of its edges, whereas a Hamiltonian walk can be extended into a Hamiltonian circuit only if its end points are adjacent. This implies that the probability that the two end points of a walk are adjacent is

$$p_{\text{adj}} = \frac{C_0 L^d}{C_1}. \quad (4.7)$$

In two dimensions, $p_{\text{adj}}$ for $L \times L$ squares can be computed from tables 2 and 3. The resulting numerical values are displayed in table 5. Note that $p_{\text{adj}}$ vanishes for odd $L$ (as it does on any bipartite lattice having an odd number of vertices).

The values in table 3 have been used in [7] to test that a certain Monte Carlo algorithm for producing Hamiltonian walks did indeed give unbiased results.

Physically, one may argue that $p_{\text{adj}}$ is proportional to the probability that the two ends of an open polymer (walk) join so as to form a ring polymer (circuit).

It is tempting to try similarly to construct from the ratio of $C_1$ and $C_2$ the probability that the conformation of two chains is such that one end point of each is adjacent on the lattice. Unfortunately, this is not possible, since certain two-chains (more precisely those in which an end point of one chain is adjacent to both end points of the other chain) can be obtained from more than one one-chain by removing an internal edge in the latter.

4.3. Lee–Yang zeros

The study of phase transitions through the location of partition function zeros in the complex magnetic field plane was initiated by Yang and Lee [16]. In particular, these authors established
that for the Ising model these zeros lie on the unit circle in terms of the variable $x = e^{2H}$, i.e., they correspond to purely imaginary values of the field $H$. The zero closest to the positive real axis is denoted as $e^{\theta_c}$, where $\theta_c$ is the so-called Lee–Yang edge. At the critical temperature, $\theta_c \to 0$ in the thermodynamic limit, and its finite-size scaling permits us to access a critical exponent. Another possible approach is to study the density of zeros $g(\theta)$. Creswick and Kim [17] have shown that at the critical temperature $g(\theta) \sim |\theta|^{1/\delta}$ for $\theta \ll 1$.

We have studied the zeros of the partition function (1.1) in terms of the variable $y = -H^2$ for $L \times L$ squares with $L \leq 12$. For odd $L$ there is one trivial zero at $y = 0$ (since $C_0 = 0$), and for even $L$ the two zeros closest to $y = 0$ form a complex conjugate pair with an imaginary part that tends to zero as $L \to \infty$. Disregarding these ‘exceptional’ zeros, all the remaining zeros (for $L$ of any parity) are found to lie on the positive real axis in the complex $y$-plane, corresponding to purely imaginary $H$ as in the Lee–Yang theorem.

We now define a finite-$L$ approximation to the density of zeros in the point $y_n$ as $g(y_n) = \frac{1}{y_n - y_{n+1}}$, where we have arranged the zeros of $Z(L \times L)$ in increasing order $y_1 < y_2 < \cdots < y_N$.

The approximations $g(y)$ are shown in figure 4 for $L = 9, 10, 11, 12$. One observes a clear crossover near $y = 1$, separating two regimes of power-law behaviours. For even $L$ the curves bifurcate for $y \ll 1$, which can be remedied by regrouping the zeros two by two (not shown). The power laws extracted from the largest available sizes read

$$g(y) \sim \begin{cases} y^{-0.46} & \text{for } y \ll 1 \\ y^{-1.66} & \text{for } y \gg 1 \end{cases}$$

We have no satisfying explanation for these exponents at present. The naive application of the standard scaling laws $\nu d = 2 - \alpha$ (Josephson) and $\alpha + 2\beta + \gamma = 2$ (Rushbrooke), and the results $\nu = \frac{1}{2}$ and $\gamma = \frac{11}{12}$ for the critical $y = 0$ system [5], leads to $1/\delta = -\frac{3}{229} \approx -0.0218\ldots$, which is clearly off the mark.
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References

[1] Duplantier B and David F 1988 J. Stat. Phys. 51 327
[2] Flory P J 1956 Proc. R. Soc. A 234 60
[3] Dill K A 1999 Protein Sci. 8 1166
[4] Nienhuis B 1982 Phys. Rev. Lett. 49 1062
[5] Jacobsen J L and Kondev J 1998 Nucl. Phys. B 532 635
[6] Gennes P-G de 1979 Scaling Concepts in Polymer Physics (Ithaca, NY: Cornell University Press)
[7] Oberdorf R, Ferguson A, Jacobsen J L and Kondev J 2006 Phys. Rev. E 74 051801
[8] Jacobsen J L 2007 Preprint 0709.2323
[9] Kasteleyn P W 1961 Physica 27 1209
[10] Mayer J-M, Guez C and Dayantis J 1990 Phys. Rev. B 42 660
[11] Jaeckel A, Sturm J and Dayantis J 1997 J. Phys. A: Math. Gen. 30 2345
[12] Bousquet-Mélou M, Guttmann A J and Jensen I 2005 J. Phys. A: Math. Gen. 38 9159
[13] Sloane N J A (ed) Sequence A003763 The Online Encyclopedia of Integer Sequences (http://www.research.att.com/~njas/sequences)
[14] Shakhnovich E and Gutin A 1990 J. Chem. Phys. 93 5967
[15] Pande V S, Grosberg A Y, Joerg C and Tanaka T 1994 J. Phys. A: Math. Gen. 27 6231
[16] Yang C N and Lee T D 1952 Phys. Rev. 87 404
  Yang C N and Lee T D 1952 Phys. Rev. 87 401
[17] Creswick R J and Kim S-Y 1997 Phys. Rev. E 56 2418