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Loop model with generalized fugacity in three dimensions

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Abstract. A statistical model of loops on the three-dimensional lattice is proposed and is investigated. It is O(n)-type but has loop fugacity that depends on global three-dimensional shapes of loops in a particular fashion. It is shown that, despite this nonlocality and the dimensionality, a layer-to-layer transfer matrix can be constructed as a product of local vertex weights for infinitely many points in the parameter space. Using this transfer matrix, the site entropy is estimated numerically in the fully packed limit.

1. Introduction

Loop models are interesting examples of statistical models of extended objects. They are related to the O(n) spin model [1, 2], a surface growth model [3], the self-avoiding walk [4], the protein folding problem [5], and so on. It includes the fully packed loop model [6] and the Hamiltonian cycle problem [7–9] as particular limits.

The partition function of an O(n) loop model on a lattice with N sites at the inverse temperature x is given by

$$Z_{\text{loop}}(n, x^{-1}) = \sum_{c \in \mathcal{C}} x^{\mathcal{N}_{\text{S}}(c) - N} n^{\mathcal{N}_{\text{L}}(c)} \qquad (n, x \in \mathbb{R}).$$
(1)

The summation is taken over the set C of all the non-intersecting loop configurations drawn along links of the lattice. The number of loops and that of sites visited by them are denoted by $N_L(c)$ and $N_S(c)$, respectively.

One may hope to study the model (1) by the transfer matrix approach. For $n \in \mathbb{Z}_+$, this is done in a simple way: one introduces link variables whose values are either occupied states with one of *n* colours or an unoccupied state and lets them interact on sites. A transfer matrix is written as a product of vertex weights straightforwardly.

For $n \notin \mathbb{Z}_+$, however, the partition sum (1) cannot be rewritten in terms of local degrees of freedom such as link variables in a simple way. It is not trivial to have a *local* transfer matrix[†]. I say a transfer matrix is *local* when its component is written as a product of weights each of which is determined by the local state configuration around a lattice site.

It is surprising that, in two dimensions, $n \notin \mathbb{Z}_+$ models admit a mapping onto a state sum model with a local vertex weight and thus have local transfer matrices [10–12]. In fact, by choosing $s \in \mathbb{C}$ satisfying $n = s + s^{-1}$, $Z_{loop}(n, x^{-1})$ can be written as

$$Z_{\text{loop}}(n, x^{-1}) = \sum_{c \in \mathcal{C}} x^{\mathcal{N}_{\text{S}}(c) - N} (s + s^{-1})^{\mathcal{N}_{\text{L}}(c)} = \sum_{c \in \overline{\mathcal{C}}} x^{\mathcal{N}_{\text{S}}(c) - N} \prod_{L \in \overline{\mathcal{L}}(c)} s^{\pm 1}$$
(2)

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[†] The use of the connectivity basis is discussed in section 5.4.

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where \overline{C} is the set of loop configurations with a direction associated with each loop. The set $\overline{\mathcal{L}}(c)$ consists of all the directed loops in a configuration *c*. A loop with the (counter-)clockwise direction is given a weight s^{+1} (s^{-1}). This weight can be realized by associating $s^{+1/4}(s^{-1/4})$ with each right(left)-turn site and the model can be regarded as a state sum model with a local vertex weight. This trick has made the study of two-dimensional loop models very fruitful.

Physics of loops in three dimensions is very attractive. It is realistic in the context of condensed matter physics. There has been a continuous suspicion that two-dimensional ones have missed some important ingredient in real physics, e.g. the protein folding problem. Three-dimensional loops also have rich mathematical structures. For instance, loops can be knotted or linked in three dimensions [13]. It is noted that a number of attractive proposals have been made to generalize the loop model to higher dimensions [14, 15].

The analysis of loop models and their generalizations in higher dimensions is, however, extremely hard to perform. Needless to say, the number of configurations increases considerably. For fugacity $n \notin \mathbb{Z}_+$, which includes the interesting case of the self-avoiding walk (n = 0), no way of constructing local transfer matrices is known. This is because specialties of two dimensions cannot be used to simplify problems any more. The mapping (2) makes use of the fact that a directed loop in two dimensions turns around just once either clockwise or counter-clockwise. It appears that this kind of trick never works in higher dimensions.

In this paper, I propose a model which generalizes (1) in a fashion specific to three dimensions. It is furnished with loop fugacity that depends on the global three-dimensional shape of loops. I show that, despite this generalization which makes the model even more nonlocal, a local transfer matrix for the system can be constructed for a number of choices of fugacity. These choices include the ones that give zero or non-integer weight to loops.

This paper is organized as follows. In section 2, I define a loop model in three dimensions generalizing (1). Its local transfer matrix is constructed for a family of points in the parameter space in section 3. In section 4, this transfer matrix is numerically diagonalized to yield an estimate of the site entropy in the fully packed limit $x^{-1} = 0$. In section 5, I discuss my results and their relation to combinatorial problems. In the appendix, a technical issue on the block diagonalization of the transfer matrix is addressed.

2. Generalized fugacity

I define a statistical model of loops on the three-dimensional simple cubic lattice $\mathbb{Z}^3 = \{\sum_{i=1}^3 m_i e_i \in \mathbb{R}^3 | m_i \in \mathbb{Z}\}, e_i \cdot e_j = \delta_{ij}$. The partition function is given by

$$Z_{\text{loop}}[n](x^{-1}) = \sum_{c \in \mathcal{C}} x^{\mathcal{N}_{\text{S}}(c) - N} \prod_{L \in \mathcal{L}(c)} n(A(L))$$
(3)

where $\mathcal{L}(c)$ is the set of loops in a configuration *c*. The loop fugacity *n* is now promoted to a function which depends on the shape of $L \in \mathcal{L}(c)$ through a quantity $A(L) \in \mathbb{R}$ defined below.

To define A(L), one begins with associating a closed trajectory on the unit sphere with each loop L. One picks a direction for L. On every point $x \in L \subset \mathbb{R}^3$ except for sites where L makes a turn, there is a unit tangential vector v(x) to L; it is either of $\pm e_i$, i = 1, 2, 3. One may regard v(x) as a mapping from $L \setminus (\text{'turn-sites'})$ to the unit sphere S^2 .

As one walks along L, v(x) jumps from a point to another on S^2 . One can naturally interpolate these points to define a continuous trajectory $v : L \to S^2$. One has only to declare that v(x) moves along the geodesic (of length $\frac{1}{2}\pi$) on S^2 at each turn-site. This is equivalent with smoothing a loop in neighbourhoods of turn-sites keeping it within the plane (figure 1). Then one defines A(L) to be the oriented area encircled in the right of the trajectory v(x). On



Figure 1. The definition of A(L). (a) The original loop L with a direction associated. (b) The loop smoothed at turn-sites. (c) Trajectory of the tangent vector on the unit sphere. An area of $A(L) = 2\pi$ is enclosed.

the lattice \mathbb{Z}^3 , A(L) takes values

$$A(L) = \frac{1}{2}m\pi (m \in \mathbb{Z}). \tag{4}$$

In two dimensions, the quantity A(L) takes values $\pm 2\pi$ and this signature corresponds to that of $s^{\pm 1}$ in (2). Therefore (3) incorporates an essential ingredient of three-dimensional loops and is regarded as a natural generalization of (2).

As is evident from the above construction, there is certain ambiguity for the value of A(L). First, because the trajectory is drawn on a closed surface of area 4π , A(L) is well-defined up to 4π . Second, the signature of A(L) is changed when the picked direction of L is reversed. I require that $n(\cdot)$ in (3) absorbs this ambiguity. Hence, it should satisfy

$$n(A) = n(A + 4\pi)$$
 (5)
 $n(-A) = n(A).$ (6)

Equations (4)–(6) imply that the fugacity function $n(\cdot)$ can be specified by five parameters $n(A), A = 0, \frac{1}{2}\pi, \pi, \frac{3}{2}\pi, 2\pi$.

In spite of the above restriction on n(A), the model (3) includes many interesting cases. Consider, for example, fugacity

$$n(A) = n_0 \delta_0^{(4)}(A) \tag{7}$$

with $n_0 \in \mathbb{R}$ and

$$\delta_b^{(a)}(A) = \begin{cases} 1 & \text{if } (\frac{A}{\pi} - b) \equiv 0 \mod a, \\ 0 & \text{otherwise.} \end{cases}$$
(8)

The sum in (3) is then restricted to configurations which consist only of loops with the oriented area $A \equiv 0 \mod 4\pi$. It should be interesting to compare the site entropy with that of the model with $n(A) = n_0$. It is also tempting to ask whether such an additional constraint changes the critical behaviour or not. The present case reminds one of the fully packed loop model in two dimensions. Its universality class differs from that of densely packed loop phase when the additional constraint that the loop length must be even is imposed [12, 16].

3. Transfer matrices from local vertex weights

In order to construct a local layer-to-layer transfer matrix for the loop model (3), I define a vertex model and show that it is equivalent with (3).

The local degree of freedom z of the vertex model lives on each link $\langle r, r \pm e_i \rangle$, $r \in \mathbb{Z}^3$. It takes one of three values \leftarrow, \rightarrow , and -(empty). On each site, six neighbouring link variables interact by the vertex weight W defined in figure 2, where $s(\omega)$ is a function that satisfies

$$s(A_1) \times s(A_2) = s(A_1 + A_2) \tag{9}$$

Figure 2. Vertex weights *W* for $Z_{\text{vertex}}[s](x^{-1})$.

and is specified further below. The partition function of the vertex model is

$$Z_{\text{vertex}}[s](x^{-1}) = \sum_{z=\leftarrow,\rightarrow,-} \prod_{r\in\mathbb{Z}^3} W(\{z(\langle r, r\pm e_i\rangle)\}).$$
(10)

Evidently, the partition function (10) has a local transfer matrix which is a product of W.

Now I show that (10) for an appropriate s is equivalent with (3). Because the weight W is nonzero only when there is one incoming and one outgoing arrow, contribution to the partition sum (10) comes only from the set \overline{C} of directed loop configurations:

$$Z_{\text{vertex}}[s](x^{-1}) = \sum_{c \in \overline{\mathcal{C}}} x^{\mathcal{N}_{S}(c) - N} \prod_{L \in \overline{\mathcal{L}}(c)} \left[\prod_{r \in L \cap \mathbb{Z}^{3}} s(\omega(r)) \right]$$
(11)

where $s(\omega(r))$ is the weight for the vertex at $r \in \mathbb{Z}^3$ in figure 2.

The factor in the square bracket in (11) is associated with a directed loop component L. To evaluate this quantity, it is crucial to observe that

$$A(L) = \sum_{\boldsymbol{r} \in L \cap \mathbb{Z}^3} \omega(\boldsymbol{r}).$$
⁽¹²⁾

Actually, the weight system in figure 2 is designed to have this property in [17–19] in the context of random walk with a spin factor [20,21]. Combining the properties (12) and (9), one finds that the factor in the square bracket is simply s(A(L)).

Using the same trick as that used in (2), one can further write the partition function (11) as a sum over undirected loop configurations:

$$Z_{\text{vertex}}[s](x^{-1}) = \sum_{c \in \mathcal{C}} x^{\mathcal{N}_{S}(c) - N} \prod_{L \in \mathcal{L}(c)} (s(A(L)) + s(-A(L))).$$
(13)

Therefore, if n(A) in the loop model (3) can be written as

n(

$$A) = s(A) + s(-A) \tag{14}$$

with a function s that satisfies (9), then the vertex model partition function $Z_{\text{vertex}}[s](x^{-1})$ defined above is equal to (3).

The requirement (9) together with the restrictions (4)–(6) on n(A) forces s(A) to have a simple form:

$$s(A) = e^{iJA} \tag{15}$$

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Table 1. The generalized fugacity *n* which generates the semigroup of allowed models. The function $\delta_{b}^{(a)}(\cdot)$ is defined in equation (8).

 $\begin{array}{ll} J & n(\cdot) \\ \hline \\ 0 & 2\delta_0^{(1/2)}(\equiv 2) \\ \frac{1}{2} & 2(\delta_0^{(4)} - \delta_2^{(4)}) + \sqrt{2}(\delta_{1/2}^{(4)} + \delta_{7/2}^{(4)} - \delta_{3/2}^{(4)} - \delta_{5/2}^{(4)}) \\ 1 & 2(\delta_0^{(2)} - \delta_1^{(2)}) \\ \frac{3}{2} & 2(\delta_0^{(4)} - \delta_2^{(4)}) - \sqrt{2}(\delta_{1/2}^{(4)} + \delta_{7/2}^{(4)} - \delta_{3/2}^{(4)} - \delta_{5/2}^{(4)}) \\ 2 & 2(\delta_0^{(1)} - \delta_{1/2}^{(1)}) \\ 0' & \delta_0^{(1)}(\equiv 1) \\ 2' & \delta_0^{(1)} - \delta_{1/2}^{(1)} \end{array}$

with $J \in \mathbb{Z}/2$. It is enough [17] to consider the cases $J = 0, \frac{1}{2}, 1, \frac{3}{2}$ and 2 because of (4). Hereafter, one introduces a shorthand notation:

$$Z_J(x^{-1}) = Z_{\text{loop}}[n(A) = e^{iJA} + e^{-iJA}](x^{-1}).$$
(16)

The vertex weights at J = 0 and 2 enjoy a special property $s(\omega) = s(-\omega)$. This enables one to define a model with only two microscopic states \leftrightarrow and -:

$$Z'_{\text{vertex}}[s](x^{-1}) = \sum_{z = \leftrightarrow, -} \prod_{r \in \mathbb{Z}^3} W(\{z(\langle r, r \pm e_i \rangle)\})$$
$$= \sum_{c \in \mathcal{C}} x^{\mathcal{N}_{S}(c) - N} \prod_{L \in \mathcal{L}(c)} s(A(L))$$
(17)

which I denote by $Z_{0'}$ and $Z_{2'}$.

The fugacity functions corresponding to $J = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, 0'$ and 2' are listed in table 1. They indeed give $n(A) \leq 0$ or $n(A) \notin \mathbb{Q}$ for some loops.

Although only a finite number of vertex models $J = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, 0'$ and 2' have been constructed above, it is possible to construct an infinite number of ones by taking the direct sum of the space of their microscopic states. More precisely, one generalizes the link variable to take one of 2q + 1 ($q \in \mathbb{Z}_+$) states: $\leftarrow_k, \rightarrow_k$ with the k labelling colours $k = 1, \ldots, q$ and an uncoloured empty state -. Introducing parameters $J_k \in \{0, \frac{1}{2}, 1, \frac{3}{2}, 2\}$, the vertex weight assignments in figure 2 are supplemented by additional rules:

- If the both two arrows have the *k*th colour, then $W = e^{iJ_k\omega}$.
- If the two colours do not agree, W = 0.

The cases $J_k = 0', 2'$ are handled in the obvious manner.

The fugacity of the 'direct sum' model $Z_{J_1 \oplus J_2 \oplus \cdots \oplus J_q}$ is simply the sum:

$$n(A) = \sum_{k=1}^{q} [(e^{iJ_k A} + e^{-iJ_k A}) \times B(J_k)]$$
(18)

$$B(J) = \begin{cases} 1 & (J = 0, \frac{1}{2}, 1, \frac{3}{2}, 2), \\ \frac{1}{2} & (J = 0', 2'). \end{cases}$$
(19)

One immediately notices that

$$Z_{0'\oplus 0'} = Z_0 \qquad Z_{2'\oplus 2'} = Z_2.$$
 (20)

Thus the fugacity functions expressible via vertex models form an infinite semigroup under addition[†] generated by $J = 0', \frac{1}{2}, 1, \frac{3}{2}$ and 2'.

[†] This direct sum operation may be used for the lattice construction [17–19] of higher-spin three-dimensional field theories.

One can also take the 'tensor product' of the space of microscopic states of Z_{J_1} and Z_{J_2} to define a model $Z_{J_1 \otimes J_2}$. Let the link variable take five values $(z_1, z_2) = \uparrow \uparrow, \uparrow \downarrow, \downarrow \uparrow, \downarrow \downarrow$, and ||. The vertex weight *W* is defined to be the product of *W* with $J = J_1$ and J_2 . Then the loop fugacity becomes

$$n(A) = [(e^{iJ_1A} + e^{-iJ_1A}) \times B(J_1)] \times [(e^{iJ_2A} + e^{-iJ_2A}) \times B(J_2)].$$
(21)

However, a new fugacity function cannot be realized because the partition function $Z_{J_1 \otimes J_2}$ is equivalent with an appropriate direct sum

$$Z_{J_1 \otimes J_2} = Z_{\overline{J}_1 \oplus \dots \oplus \overline{J}_q} \tag{22}$$

corresponding to the decomposition rule of the representation of SU(2).

4. Entropy estimates

I numerically diagonalize the transfer matrices constructed in section 3. Throughout this section, I concentrate on the fully packed limit $x^{-1} = 0$ where all the sites are visited by a loop. This simple case is in fact a very interesting case; in two dimensions, this limit yields a new universality class with a shifted central charge on several bipartite lattices and has been attracting much attention [16,22–24]. It would be interesting to look at the limit where the two strong constraints are combined: the fully packing constraint $x^{-1} = 0$ and the constraint (7) on the shape of loops.

The site entropy in the thermodynamic limit is defined by

$$f[n](\infty) = \lim_{N \to \infty} \frac{1}{N} \log Z_{\text{loop}}[n](x^{-1} = 0).$$
(23)

I evaluate this quantity on quasi-one-dimensional geometry $L_1 \times L_2 \times L_3$, $L_3 \rightarrow \infty$ while L_1 , L_2 are kept finite by calculating the largest eigenvalue of the transfer matrix in an appropriate sector.

Let *T* be the layer-to-layer transfer matrix in $+e_3$ (vertical) direction for the vertex model defined in (10). Then *T* acts on linear combinations of arrays of $L_1 \times L_2$ vertical (coloured) arrows. One can take either hard-wall or periodic boundary condition in the horizontal directions.

It is important to note that the transfer matrix T commutes with the operator giving the net flow of arrows of *k*th colour in $+e_3$ direction:

$$d_k = (\# \uparrow_k) - (\# \downarrow_k) \tag{24}$$

which is understood as

$$d_k = (\# \updownarrow_k) \bmod 2 \tag{25}$$

for $J_k = 0'$ and 2'. Thus T is block diagonalized as

$$T = \bigoplus_{d} T_d \qquad d = (d_1, \dots, d_q).$$
⁽²⁶⁾

The quantity (23) is obtained as

$$f[n](\infty) = \lim_{L_1, L_2 \to \infty} \frac{1}{L_1 L_2} \log |\lambda_0^0(L_1, L_2)|$$
(27)

where $\lambda_d^i(L_1, L_2)$ is the *i*th largest eigenvalue of $T_d(L_1, L_2)$. The condition d = 0 excludes unwanted configurations that have unbalanced arrows travelling along the infinite direction.

J	$2 \times 2(h)$	$3 \times 3(h)$	$3 \times 4(h)$	2 × 2(p)	3 × 3(p)	3 × 4(p)	$4 \times 4(p)$				
0	0.542 024 95	0.591 454 47	0.635 240 92	1.058 512 6	0.838 416 78	0.833 401 28	_				
$\frac{1}{2}$	0.271 236 80	0.33576248	0.350 509 51	0.794 513 46	0.559 000 63	0.558 959 24	_				
ĩ	0.515 859 27	0.502 347 91	0.556 462 23	0.971 704 02	0.698 126 31	0.698 320 61	_				
$\frac{3}{2}$	0.355 923 18	0.359 081 94	0.371 368 01	0.794 513 46	0.574 359 35	0.494 963 87	_				
2	0.494 996 47	0.454 689 72	0.516 154 98	1.0406166	0.662 007 16	0.674 409 81	_				
0′	0.462 989 39	0.556 506 97	0.600 729 54	0.91847381	0.796 317 88	0.801 357 60	0.81947983				
2′	0.38697370	0.37695844	0.422 725 84	0.87898824	0.556 089 04	0.584 974 12	0.609 319 46				

Table 2. The site entropy estimated numerically. $L_1 \times L_2$ is the size of a layer while (p) and (h) mean periodic and hard-wall boundary conditions in a layer.

Shown in tables 2 and 3 are the finite- L_1 , L_2 results[†]. The asymmetric Lanczos algorithm is utilized for the present sparse eigenproblem.

The obstacle in making L_1 and L_2 large in the actual numerical work is of course the exponential growth of the dimensionality of the transfer matrix. The selection of d = 0 sector helps to reduce the dimensionality, though the improvement is polynomial. For a direct sum $Z_{J_1 \oplus \dots \oplus J_a}$, the dimensionality is estimated to be

dim
$$(d = 0 \text{ sector}) \sim (1 + 2u + p)^{L_1 L_2} \times 2^{-p} \left(\frac{3}{4\pi L_1 L_2}\right)^{u/2}$$
 (28)

where $p = \#\{k | J_k = 0' \text{ or } J_k = 2'\}$, u = q - p. One notices that it is better to recast $Z_{2' \oplus 2'}$ as Z_2 if one is interested in its d = 0 sector.

The exponential growth is severe even after restricting to the d = 0 sector. In order to increase L_1L_2 as much as possible within the available computer resources, I have further decomposed T_0 with respect to the eigenvalue of shift (lattice momentum) operator for the periodic boundary case where the translational symmetry is present. I have looked at the zero-momentum sector $T_0^{(0,0)}$ as described in the appendix. It is quite natural to expect that the largest eigenvalue lies there. By this decomposition, the dimensionality of the eigenproblem is reduced, at most, by $(L_1L_2)^{-1}$. As a drawback, the matrix $T_0^{(0,0)}$ becomes less sparse than the original T_0 . With both effects combined, some improvements in the memory usage and the CPU time are observed. Thus the analysis of larger systems becomes possible for the periodic boundary case, as seen in tables 2 and 3.

5. Discussions

In the comparison between the periodic and the hard-wall boundary conditions, one notices that the periodic case always has larger site entropy. This is because many of the loops that wind nontrivially in the horizontal directions satisfy A(L) = 0 and the loops with A(L) = 0 contribute to every partition sum with a positive fugacity.

The numerical works in this study have been carried out on modest workstations. Unfortunately, information in the thermodynamic limit $L_1, L_2 \rightarrow \infty$ is out of reach in the present analysis. For the study of criticality, [17], where random walks with the weight in figure 2 are studied, is quite suggestive. It is reported that Euclidean symmetry is not always recovered even in the continuum limit.

I discuss relations with combinatorial problems below.

5.1. Even and odd number of loops of a specific type

For most allowed values of *J*, the loop fugacity takes both positive and negative values. Some interesting combinatorial information is encoded in these models. For example, the linear combinations $\frac{1}{2}(Z_{0'} \pm Z_{2'})$ counts the number of loop configurations such that there are even (odd) number of loops for which $\frac{2}{\pi}A(L) \equiv 1 \mod 2$, e.g.,

$$\frac{1}{2}(Z_{0'} \pm Z_{2'}) = \begin{cases} \sum_{c \in \mathcal{C}_{\text{even}, \frac{1}{2}}} 1, \\ \sum_{c \in \mathcal{C}_{\text{odd}, \frac{1}{2}}} 1 \end{cases}$$
(29)

† I have also measured several leading eigenvalues of T_d with $d = (d_1, \ldots, d_q)$, $d_k = 0, \pm 1$. These are related to correlation length of operators in the theory. These results will be reported elsewhere.

	12	2 > 2(h)	$3 \times 3(h)$	$2 \times 2(n)$	$3 \times 3(n)$	$3 \times 1(h)$	$3 \times I(n)$
$\Phi_k J_k$	n	2 × 2(11)	5 × 5(II)	2 × 2(p)	3 × 3(þ)	5 × 4(II)	3 × 4(þ)
$0'\oplus 2'$	$2\delta_0^{(1)}$	0.523 305 15	0.573 909 34	1.050 2400	0.815 036 26	0.619 355 81	0.81580656
$0 \oplus 0$	4	0.644 981 33	0.650 207 10	1.235 4255	0.90747958	_	_
$0 \oplus 2$	$4\delta_0^{(1)}$	0.633 314 28	0.627 658 33	1.232 054	0.88008432	_	_
$0'\oplus 2'\oplus 1$	$4\delta_0^{(2)}$	0.632 161 04	0.616 640 18	1.2110124	0.861 217 44	_	_
$0 \oplus 0 \oplus 0 \oplus 0$	8	0.769 110 76		1.450 1153	1.010 833 8	—	—
$0 \oplus 0 \oplus 2 \oplus 2$	$8\delta_0^{(1)}$	1.3280134		1.4490048	0.98982172	_	_
$0 \oplus 1 \oplus 1 \oplus 2$	$8\delta_0^{(2)}$	0.75985245		1.4364447	0.97947213	_	_
$0' \oplus 2' \oplus \frac{1}{2} \oplus 1 \oplus \frac{3}{2}$	$8\delta_0^{(4)}$	0.364 649 34		1.3863922	0.88604978	_	_
$\frac{1}{2} \oplus \frac{3}{2}$	$4(\delta_0^{(4)} - \delta_2^{(4)})$	0.47382047	0.417 706 63	1.0397208	0.636 308 00	_	_
$\overline{0} \oplus \frac{1}{2}$	¢ℚ	0.400 131 09	0.546 704 71	1.168 6609	0.846 525 98	_	_
$0 \oplus \frac{3}{2}$	$\notin \mathbb{Q}$	0.44457252	0.55636026	1.168 6609	0.846 943 06	_	_
$0' \oplus \overline{0} \oplus \frac{1}{2}$	¢ℚ	0.480 945 69	0.57807813	1.252 0659	0.627 959 92	—	—

Table 3. The site entropy estimated numerically. $L_1 \times L_2$ is the size of a layer while (p) and (h) mean periodic and hard-wall boundary conditions in a layer.



Figure 3. When u_0 , the tangent vector at $v(x_0)$, is parallel-transported along the trajectory on S^2 , it receives holonomy whose magnitude (angle θ) is equal to the oriented area A(L) the path encloses.

where $C_{\text{even(odd)},a}$ is the subset of C and is defined by the following properties:

- $c \in C_{\text{even(odd)},a}$ contains even (odd) number of loops with $A(L)/a\pi \equiv 1 \mod 2$.
- All other loops in $c \in C_{\text{even(odd)},a}$ satisfy $A(L)/a\pi \equiv 0 \mod 2$.

Similarly, the quantities $\frac{1}{2}(Z_{0'\oplus 2'}\pm Z_1)$ and $\frac{1}{2}(Z_{0'\oplus 2'\oplus 1}\pm Z_{\frac{1}{2}\oplus\frac{3}{2}})$ are interpreted as the sums over $\mathcal{C}_{even(odd),1}$ and $\mathcal{C}_{even(odd),2}$.

Of the two Z in (29), the one with the larger leading eigenvalue dominates the sum in the limit $L_3 \rightarrow \infty$ studied in section 3. In finite geometries, both terms contribute to yield an exact number.

5.2. Self-avoiding walk

The partition function (1) in the limit $n \rightarrow 0$ corresponds to the enumeration of selfavoiding walks. Self-avoiding walks in three dimensions have mainly been studied by the exact enumeration method due to the lack of transfer matrix formalism as pointed out in the introduction.

The model I propose in this paper can be regarded as a step forward to overcome this difficulty; in the models $Z_{0'\oplus 2'}$, $Z_{0'\oplus 2'\oplus 1}$ and $Z_{0'\oplus 2'\oplus \frac{1}{2}\oplus 1\oplus \frac{3}{2}}$, the fugacity is set zero for families of loops. This is, however, achieved at the cost of having larger n for another family of loops. Within the present construction, loops with $A(L) \equiv 0 \mod 4\pi$ cannot have weights different from the number of possible link states. Thus the partition function listed above serve only as a very loose upper bound for the entropy of self-avoiding walks.

The problem of construction of a local transfer matrix to enumerate self-avoiding walks on three-dimensional lattices still remains open.

5.3. Mapping to ribbon configurations

The oriented area defined in (3) has a nice geometric interpretation as holonomy. The tangent vector v(x) moves along a trajectory on S². Let the unit vector tangential to this trajectory at $v(x_0)$ be u_0 (figure 3). Consider the parallel transport (in the sense of Riemannian geometry) of u_0 along the trajectory v(x) on S^2 .

When u_0 is transported back to $v(x_0)$, it gains some holonomy (the angle θ in figure 3). This holonomy angle is given by the integration of the scalar curvature of S^2 over the domain encircled by the trajectory and is nothing but the oriented area A(L). In the real space $\mathbb{Z}^3 \subset \mathbb{R}^3$, the holonomy described above is nicely kept track of by broadening the loop segment to a 'ribbon' with the distinction of the right and the reversed sides. The parallel transportation can

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Figure 4. Examples of allowed ways of bending ribbons at sites (except for the ones indicated by grey arrows). The holonomy is accumulated at the sites indicated by grey arrows. The right and the reverse sides of ribbons are represented by white and black colours.

be recasted as a rule of bending ribbons on sites, which is shown in figure 4. Among the loop configurations shown in figure 4, the partition sum Z_{loop} with fugacity $n = \delta_0^{(2)}$, $\delta_0^{(1)}$ and $\delta_0^{(1/2)}$ receives contribution from {(a)}, {(a), (b)}, and {(a), (b), (c)}, respectively.

For $n = 4\delta_0^{(2)}$, the sum in (3) is over ribbon loop configurations without mismatch. In that interpretation, the coefficient four is naturally regarded as the number of directions the right side can face. Therefore, $Z_{\text{loop}}[n = 4\delta_0^{(2)}](x^{-1})$ is nothing but the generating function of the number of allowed ribbon configurations[†].

Similarly, the partition sum for $n = 2\delta_0^{(1)}$ can be interpreted as the sum over the configurations of ribbons without the distinction between the right and the reverse sides, while in the case $n = \delta_0^{(1/2)}$, the loop segment is just a chord. This interpretation suggests that (3) may be regarded as a model of polymers with various partially broken axial symmetry by, for instance, the presence of side chains.

5.4. Comparison with the connectivity basis

The connectivity basis [25, 26] is very powerful in that one can always write a transfer matrix for a loop model with respect to it. It has been very useful for numerical calculation in two dimensions.

Nevertheless, I have avoided the use of the connectivity basis in this paper. The reason is the following. First, its fundamental degrees of freedom are not the link variables and the transfer matrix with respect to it is not local. Local transfer matrices have merits even in two dimensions. Namely, it paved the way to the Bethe ansatz solution [27, 28] and the conformal field theoretic description [29,30] via Coulomb gas representation. Second, in three dimensions and higher, the size of connectivity basis grows considerably because of the lack of the planarity constraint. It is not clear if it is effective to perform numerical calculation in this basis. In two dimensions, the present basis is as good as the connectivity one [12,22].

I suppose it is very important to see how useful the connectivity basis in three dimensions is and to try to improve the efficiency of the calculation in that basis.

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[†] This observation clearly indicates a simple way of constructing transfer matrices for this fugacity function. The link variable represents the ribbon which can be placed in four ways. The rule of bending is implemented in the vertex weight. The construction in section 3, however, has an advantage: the size of the matrix can be reduced more by the choice of the sector d = 0.

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Appendix. Projection to zero momentum subspace

In this short note, I describe the block diagonalization of the transfer matrix with respect to the eigenvalues of the lattice momentum operators. The zero-momentum subspace and a reduced transfer matrix which acts on it are explicitly constructed[‡].

One may start with the $(2q + 1)^{L_1L_2}$ -dimensional whole space of coloured arrow configurations or an eigenspace of the operator d. One considers the matrix elements in the basis u_i , (i = 1, ..., m), each of which represents a single arrow configuration such as $\uparrow \downarrow \mid \cdots \uparrow \mid \downarrow$:

$$Tu_{i} = \sum_{j=1}^{m} T_{i}^{j} u_{j}.$$
(30)

In this natural basis, the matrix T becomes sparse.

Let S_1 and S_2 be discrete shift operators in the horizontal directions. Then the vectors

$$v_j = \sum_{a=0}^{L_1 - 1} \sum_{b=0}^{L_2 - 1} (S_1)^a (S_2)^b u_j$$
(31)

are zero-momentum ones.

One classifies the index set as $\{1, \ldots, m\} = \bigsqcup_{I=1}^{M} V_I$ by an equivalence relation $i \sim j \Leftrightarrow v_i = v_j$. Then $I = 1, \ldots, M$ labels the zero-momentum subspace. The (I, J)-component of the block matrix is simply

$$(T_{\mathbf{0}}^{(0,0)})_{I}^{J} = \sum_{j \in V_{J}} T_{i}^{j} \qquad (i \in V_{I}).$$
(32)

This procedure is fairly easy to implement in the sparse algorithm.

Evidently, a slight modification of the above procedure enables one to focus on a chosen nonzero momentum subspace. It will be useful for identifying excited states.

It is noted that the above block decomposition can be applied even if the seam factor is present, e.g. to two-dimensional O(n) model with cylinder topology. One can make the system translationally invariant by distributing the seam factor among all horizontal links. I have checked that this prescription improves the efficiency of the the enumeration of Hamiltonian cycles performed in [22] although the weight system becomes system-size dependent.

References

- Nienhuis B 1982 Exact critical point and critical exponents of O(n) model in two dimensions *Phys. Rev. Lett.* 49 1062
- [2] Domany E, Mukamel D, Nienhuis B and Schwimmer A 1981 Duality relations and equivalences for models with O(n) and cubic symmetry Nucl. Phys. B 190 279
- [3] Kondev J and Henley C L 1995 Four-colouring model on the square lattice: a critical ground state *Phys. Rev.* B 52 6628
- [4] Duplantier B and Saleur H 1987 Exact critical properties of two-dimensional dense self-avoiding walks Nucl. Phys. B 290 291

† It may well improve the efficiency just to choose a zero-momentum state as the initial Lanczos vector in the sparse algorithm without explicitly constructing a transfer matrix in the subspace as is done in the text.

- [5] Chan H S and Dill K A 1989 Compact polymers Macromolecules 22 4559
- [6] Blöte H W J and Nienhuis B 1994 Fully packed loop model on the honeycomb lattice *Phys. Rev. Lett.* **72** 1372
 [7] Orland H, Itzykson C and de Dominicis C 1985 An evaluation of the number of Hamiltonian paths *J. Physique*
- **46** L353
- [8] Suzuki J 1988 Evaluation of the connectivity of Hamiltonian paths on regular lattices J. Phys. Soc. Japan 57 687
- [9] Higuchi S 1998 Field theoretic approach to the counting problem of Hamiltonian cycles of graphs *Phys. Rev.* E 58 128
 - (Higuchi S 1997 Preprint cond-mat/9711152)
- [10] Baxter R J 1970 Colourings of a hexagonal lattice J. Math. Phys. 11 784
- [11] Nienhuis B 1987 Coulomb gas formulation of two-dimensional phase transitions Phase Transitions and Critical Phoenomena vol 11, ed C Domb and J Lebowitz (New York: Academic) pp 1–53
- [12] Batchelor M T, Blöte H W J, Nienhuis B and Yung C M 1996 Critical behaviour of the fully packed loop model on the square lattice J. Phys. A: Math. Gen. 29 L399
- [13] Nechaev S K 1996 Statistics of Knots and Entangled Random Walks (Singapore: World Scientific) (Nechaev S K 1998 Preprint cond-mat/9812205)
- [14] Wiese K J and Kardar M 1998 A geometric generalization of field theory to manifolds of arbitrary dimension Eur. Phys. J. B 7 187

(Wiese K J and Kardar M 1998 Preprint cond-mat/9803279)

- [15] Wiese K J and Kardar M 1998 Generalizing the O(N)-field theory to N-coloured manifolds of arbitrary internal dimension D Nucl. Phys. B 528 469
 (Wiese K J and Kardar M 1998 Preprint cond-mat/9803389)
- [16] Jacobsen J L 1999 On the universality of compact polymers J. Phys. A: Math. Gen. 32 5445 (Jacobsen J L 1999 Preprint cond-mat/9903132)
- [17] Asano M, Itoi C and Kojima S-I 1995 Random walk construction of spinor fields on three-dimensional lattice Nucl. Phys. B 448 533
 - (Asano M, Itoi C and Kojima S-I 1994 Preprint hep-th/9412215)
- [18] Asano M, Itoi C and Kojima S-I 1994 Quantum diffusion process with a complex weight on three-dimensional lattice Proc. Int. Seminar Devoted to the 140th Birthday of Henri Poincaré (IHPE Protovino, Russia) Preprint hep-th/9410090
- [19] Itoi C 1994 Smooth paths on three-dimensional lattice *Phys. Rev. Lett.* **73** 3335 (Itoi C 1994 *Preprint* hep-th/9406123)
- [20] Polyakov A M 1988 Fermi-Bose transmutations induced by gauge fields Mod. Phys. Lett. A 3 325
- [21] Iso S, Itoi C and Mukaida H 1990 Geometric description for spinning particles in three dimensions and Chern– Simons–Polyakov theory *Phys. Lett.* B 236 287
- [22] Higuchi S 1999 Compact polymers on decorated square lattices J. Phys. A: Math. Gen. 32 3697 (Higuchi S 1998 Preprint cond-mat/9811426)
- [23] Di Francesco P, Guitter E and Kristjansen C 1999 Fully packed O(n = 1) model on random Eulerian triangulations *Nucl. Phys.* B **549** 657
 - (Di Francesco P, Guitter E and Kristjansen C 1999 Preprint cond-mat/9902082)
- [24] Guitter E, Kristjansen C and Nielsen J L 1999 Hamiltonian cycles on random Eulerian triangulations Nucl. Phys. B 546 731
 - (Guitter E, Kristjansen C and Nielsen J L 1998 Preprint cond-mat/9811289)
- [25] Schmalz T G, Hite G E and Klein D J 1984 Compact self-avoiding circuits on two-dimensional lattices J. Phys. A: Math. Gen. 17 445
- [26] Blöte H W J and Nienhuis B 1989 Critical behaviour and conformal anomaly of the O(n) model on the square lattice J. Phys. A: Math. Gen. 22 1415
- [27] Baxter R 1982 Exactly Solvable Models in Statistical Mechanics (London: Academic)
- [28] Batchelor M T and Blöte H W 1988 Conformal anomaly and scaling dimensions of the O(n) model from an exact solution on the honeycomb lattice Phys. Rev. Lett. 61 138
- [29] Cardy J 1994 Geometrical properties of loops and cluster boundaries *Fluctuating Geometries in Statistical Mechanics and Field Theory (Les Houches Session 62)* ed F David *et al* (Amsterdam: Elsevier) (Cardy J 1994 *Preprint* cond-mat/9409094)
- [30] Jacobsen J L and Kondev K 1998 Field theory of compact polymers on the square lattice Nucl. Phys. B 532 635 (Jacobsen J L and Kondev K 1998 Preprint cond-mat/9804048)