Planar lattice gases with nearest-neighbour exclusion.

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Abstract

We discuss the hard-hexagon and hard-square problems, as well as the corresponding problem on the honeycomb lattice. The case when the activity is unity is of interest to combinatorialists, being the problem of counting binary matrices with no two adjacent 1’s. For this case we use the powerful corner transfer matrix method to numerically evaluate the partition function per site, density and some near-neighbour correlations to high accuracy. In particular for the square lattice we obtain the partition function per site to 43 decimal places.

1 Introduction

Partition function of hard squares

In recent years there has been interest amongst combinatorialists in the problem of counting the number of “legal matrices” [3, 10, 11, 12]. These are matrices whose elements are either 0 or 1. Two elements are said to be ‘adjacent’ if they lie in positions \((i, j)\) and \((i + 1, j)\), or if they lie in positions \((i, j)\) and \((i, j + 1)\). No two 1’s are allowed to be adjacent.

In statistical mechanics this is known as the ‘hard squares’ problem: how many ways are there of putting particles on a square lattice of \(N\) sites so that no two share the
same site, or are adjacent. (An economical way of formulating this rule is to say that there is at most one particle on every edge.)

In statistical mechanics we usually generalize this problem by specifying the number of particles. Thus we might define $g(m, N)$ to be the number of ways of putting $m$ particles on a given lattice of $N$ sites, subject to the above exclusion rule. This is the ‘canonical’ partition function. The ‘grand canonical partition function’ is

$$\Xi_N(z) = \sum_m g(m, N) z^m , \quad (1)$$

$z$ being an arbitrary real (or complex) variable. For $z$ real and positive we expect on physical grounds that the limit

$$\kappa(z) = \lim_{N \to \infty} [\Xi_N(z)]^{1/N} \quad (2)$$

will exist and be independent of the shape of the lattice, so long as the shape is not pathological - it must certainly become infinite in all directions.

It follows that what combinatorialists are interested in is $\Xi_N(1)$ and $\kappa(1)$. While the function $\kappa(z)$ has been extensively investigated, by series expansions and numerically [7, 18, 25, 26], less attention has been paid by statistical mechanics to its value at $z = 1$. Estimates for $\kappa(1)$ of $1.5030$ and $1.503048082$ are given in [23] and [24], and lower and upper bounds of $1.503263$ and $1.517513$ in [21].

Amongst combinatorialists, Engel [12] obtained the estimate $1.50304808$, and Calkin and Wilf [9] have recently obtained $1.5030480824753323$, with rigorous lower and upper bounds $1.503047782$ and $1.5035148$. This estimate has been refined by McKay to $1.50304808247533226$ [22].

Here we use the corner transfer matrix method to calculate $\kappa(1)$ and various related quantities and obtain the result $1.503048082475332264322066329475536893857810$. Based on the observed convergence of the sequence of successive approximations (and on the expected error of $A^4_{49}$), we believe this result to be correct to the 43 decimal places given.
Related models and quantities

For the corresponding problem on the triangular lattice, known as ‘hard hexagons’, Metcalf and Yang in 1978 [23] conjectured that \( \log \kappa(1) = 1/3 \). This intriguing conjecture prompted Baxter and Tsang [8] to obtain more accurate numerical values, using the corner transfer matrix method [3]. They disproved Metcalf and Yang’s conjecture, but as a result the author stumbled on the fact that the problem could be solved exactly by the ‘Yang-Baxter’ method (C.N. Yang, rather than his brother C.P.). [2, 5]

For the square and honeycomb lattices, the problem has not been solved exactly and the suggestive clues of hard hexagons are missing. Even so, the method provides a powerful way of calculating \( \kappa(1) \) to considerable numerical precision. We do this here, obtaining it to 42 and 39 decimal places for the square and honeycomb lattices, respectively. For completeness, we also evaluate \( \kappa(1) \) for the triangular lattice, using the known exact result, and give it here to 55 decimal places.

A related quantity is the density, or probability that a given site is occupied:

\[
\rho(z) = \Xi_N(z)^{-1} \sum_m (m/N) g(m, N) z^m = z \frac{d}{dz} \ln \kappa(z) , \tag{3}
\]

also expected to tend to a limit for a large lattice. This is a ‘single-site’ property and is also readily calculated by the corner transfer matrix method, so we present numerical values for \( \rho(1) \) here, along with some next-nearest neighbour correlation results.

It should be noted that the models are expected to undergo a phase transition from a disordered fluid phase to an ordered solid crystalline phase at \( z = 11.09017... \), 3.7962..., 7.92..., \( \rho = 0.27639... \), 0.368..., 0.422..., for the triangular, square and honeycomb lattices, respectively. [2, 4, 27]. For each lattice, these critical values of \( z \) are considerably greater than \( z = 1 \), so the gas is well and truly in the fluid phase and we expect successive finite truncations of the corner transfer matrix equations (with no sub-lattice symmetry breaking) to converge rapidly, and indeed we observe this. The method converges more slowly as \( z \) approaches the critical value.
2 Low density series expansions

The series expansions were obtained for these models in the sixties \cite{17, 18, 28} to orders $z^8, z^{13}, z^{13}$, respectively. They have since been extended, e.g. in \cite{4, p. 408}, \cite{7}. Here we give each to order $z^{13}$:

- **triangular**:
  \[
  \kappa = 1 + z - 3 z^2 + 16 z^3 - 106 z^4 + 789 z^5 - 6318 z^6 + 53198 z^7 - 464673 z^8 + 4174088 z^9 - 38332500 z^{10} + 358371345 z^{11} - \\
  3400238419 z^{12} + 32664062740 z^{13} + O(z^{14})
  \]

- **square**:
  \[
  \kappa = 1 + z - 2 z^2 + 8 z^3 - 40 z^4 + 225 z^5 - 1362 z^6 + 8670 z^7 - 57253 z^8 + 388802 z^9 - 2699202 z^{10} + 19076006 z^{11} - \\
  136815282 z^{12} + 993465248 z^{13} + O(z^{14})
  \] (4)

- **honeycomb**:
  \[
  \kappa^2 = 1 + 2 z - 2 z^2 + 6 z^3 - 23 z^4 + 100 z^5 - 469 z^6 + 2314 z^7 - 11841 z^8 + 62286 z^9 - 334804 z^{10} + 1831358 z^{11} - \\
  10162679 z^{12} + 57080840 z^{13} + O(z^{14})
  \]

3 Corner transfer matrix equations

Label the sites of the lattice $i = 1, \ldots, N$. With site $i$ associate an occupation number (or spin) $\sigma_i$, with value 0 if the site is empty, 1 if it is full. Then for all three lattices the partition function is

\[
\Xi_N(z) = \sum \prod_i z^{\sigma_i} \prod_{<ij>} e(\sigma_i, \sigma_j) ,
\] (5)
where the sum is over all values 0 or 1 of all the occupation numbers (without restriction), the second product is over all edges \(<i,j>\) of the lattice, and

\[
e(0,0) = e(0,1) = e(1,0) = 1, \quad e(1,1) = 0.
\]

(6)

For the \textit{triangular} lattice the corner transfer matrix equations are given in \([8]\). They are

\[
\sum_b F(a,b)A^2(b)F(b,a) = \xi A^4(a),
\]

\[
\sum_c w(a,b,c)F(a,c)A(c)F(c,b) = \eta A(a)F(a,b)A(b),
\]

(7)

\[
\kappa = \eta^2 / \xi .
\]

Here \(a, b, c\) are site occupation numbers, taking the values 0 or 1, and \(w(a,b,c)\) is the weight function of a triangular face of the lattice, which for our hard molecule model is

\[
w(a,b,c) = \frac{z^{a+b+c}/6}{e(a,b)e(b,c)e(c,a)}.\]

For the \textit{square} lattice the corner transfer matrix equations are given in \([1]\) and \([8]\). Specializing to the translation-invariant case (with no symmetry breaking), they are

\[
\sum_b F(a,b)A^2(b)F(b,a) = \xi A^2(a),
\]

\[
\sum_{c,d} w(a,c,d,b)F(a,c)A(c)F(c,d)A(d)F(d,b) = \eta A(a)F(a,b)A(b),
\]

(8)

\[
\kappa = \eta / \xi ,
\]

the face weight function being

\[
w(a,b,c,d) = \frac{z^{a+b+c+d}/4}{e(a,b)e(b,c)e(c,d)e(d,a)}.
\]

For the \textit{honeycomb} lattice, we found it convenient to transform the model to one on the triangular lattice by dividing it into two sub-lattices and summing over all the spins on one sub-lattice. (This is a decimation transformation.) The resulting triangular lattice model has different face weights \(w_1, w_2\) for up-pointing and down-pointing triangles, respectively:

\[
w_1(a,b,c) = \frac{z^{a+b+c}/3 + z\delta_{a0}\delta_{b0}\delta_{c0}}{e(a,b)e(b,c)e(c,a)}, \quad w_2(a,b,c) = 1 ,
\]
and the equations (7) generalize to

\[
\sum_{b} F_i(a, b) A_i(b) A_j(b) F_j(b, a) = \xi A_j(a) A_i(a) A_j(a) A_i(a),
\]
\[
\sum_{c} w_i(a, b, c) F_i(a, c) A_i(c) F_i(c, b) = \eta_i A_j(a) F_j(a, b) A_j(b),
\]  
(9)

\[
\kappa = (\eta_1 \eta_2 / \xi)^{1/2},
\]

for \((i,j) = (1,2)\) and \((2,1)\). Here \(\kappa\) is the partition function per site of the original honeycomb lattice.

In each case \(A(a)\) is the corner transfer matrix centred on a site of occupation number \(a\). Define the matrix

\[
M(a) = A^6(a), \quad A^4(a), \quad [A_1(a) A_2(a)]^3,
\]

for the three lattices, respectively. Then the density is

\[
\rho = \text{Trace} M(1) / [\text{Trace} M(0) + \text{Trace} M(1)].
\]

Similarly, \(F(a, b)\) is the ‘half-row’ transfer matrix associated with an edge with occupation numbers \(a, b\). For this reason \(F(1,1)\) is the zero matrix for the first two lattices. (For the honeycomb lattice the decimation transformation means that \(F_i(a, b)\) is associated with next-nearest neighbour sites \(a, b\), so \(F_i(1,1)\) is not zero.) Other local occupation probabilities can be obtained by building up a face or faces of the lattice. For instance, for the square lattice the probability that two next-nearest-neighbour (i.e. diagonally adjacent) sites are simultaneously occupied is

\[
\rho_{nn} = \frac{w(1,0,1,0) \text{Trace} \left[ A(1) F(1,0) A(0) F(0,1) A(1) F(1,0) A(0) F(0,1) \right] }{ \sum_{a,b,c,d} \ w(a,b,c,d) \text{Trace} \left[ A(a) F(a,b) A(b) F(b,c) A(c) F(c,d) A(d) F(d,a) \right] } .
\]

(12)

It can be convenient to define the larger matrices

\[
A = \begin{pmatrix} A(0) & 0 \\ 0 & A(1) \end{pmatrix}, \quad F = \begin{pmatrix} F(0,0) & F(0,1) \\ F(1,0) & F(1,1) \end{pmatrix},
\]
\[
S = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad M = \begin{pmatrix} M(0) & 0 \\ 0 & M(1) \end{pmatrix}.
\]

(13)
(Generalizing as needed for the honeycomb lattice.)

These extended matrices $A$, $F$, $M$ are real and symmetric. The corner transfer matrix equations above define these matrices to within irrelevant similarity transformations: it is convenient to remove this arbitrariness by choosing $A$ and $M$ to be diagonal.

The equations are exact in the limit when the matrices are infinite-dimensional. Finite-dimensional truncations provide a sequence of rapidly converging approximations and the techniques needed to handle these are explained in [[1], [3], [8]]. For each lattice a column $k, b$ of the second equation plays the role of an eigenvalue equation, the eigenvalue being the diagonal element $k, b$ of $A$, and the eigenvector being column $k, b$ of $F$. The first equation fixes the normalization of the eigenvector. In any finite truncation there are more eigenvalues than needed: one selects those giving the larger eigenvalues of $M$. One can normalise the diagonal matrix $M$ to have maximum element unity, the diagonal elements being arranged in numerically decreasing order. These elements do not change dramatically as one increases dimensionality, so one can regard the truncation where $M$ has dimensionality $r$ as providing an approximation for the largest $r$ elements of the true infinite-dimensional matrix $M$. The magnitude of the largest element omitted provides a measure (in practice it seems a somewhat over-confident measure) of the accuracy of any given truncation.

For each lattice, and for any finite truncation, the CTM equations can be obtained from a variational principle for $\kappa$.

4 Simple approximations

Bethe approximation

A simple approximation for lattice models is to replace the lattice by a Bethe lattice (i.e. a Cayley tree with surface effects excluded) of the same coordination number $q$. Specializing the formula given in Chapter 4 of [8], we get

$$\kappa = (1 + m)/(1 - m^2)^{q/2}, \quad \rho = m/(1 + m), \quad (14)$$
where $m$ is related to $z$ by

$$z = m/(1 - m)^q .$$

(15)

This approximation is self-consistent in that the relation (3) is satisfied. When $z$ is small, so is $m$ and we readily obtain the series expansions for the three lattices (with $q = 6, 4, 3$, respectively):

$$\kappa = 1 + z - 3z^2 + 18z^3 + O(z^4) ,$$

$$\kappa = 1 + z - 2z^2 + 8z^3 - 41z^4 + O(z^5) ,$$

$$\kappa^2 = 1 + 2z - 2z^2 + 6z^3 - 23z^4 + 100z^5 - 470z^6 + O(z^7) .$$

(16)

Let $q'$ be the number of edges round a face of the lattice (this is the coordination number of the dual lattice), so $q' = 3, 4, 6$ for the three lattices, respectively. Comparing (16) with (4), we see that for each lattice the Bethe approximation fails at order $z^{q'}$, which is the order at which a circuit first makes a contribution to the partition function.

**Kramers-Wannier approximation**

A more accurate approximation, which at least in some circumstances is related to that of Kramers and Wannier [20], is to take the corner transfer matrices $A(a), F(a, b)$ in (7) - (9) to be one-by-one matrices. Then $A, F$ are two-by-two matrices. For the $\text{triangular}$ lattice this gives

$$\kappa = (1 - m)^3/(1 - 2m)^2 , \quad \rho = m/(1 + m) ,$$

(17)

where $M$ has the diagonal entries $1, m$ and

$$z = m(1 - m)^6/(1 - 2m)^6 .$$

Expanding, this gives

$$\kappa = 1 + z - 3z^2 + 16z^3 - 106z^4 + 789z^5 - 6319z^6 + O(z^7) .$$

(18)

For the $\text{square}$ lattice,

$$\kappa = (1 + t)^2/(1 + t - t^2) , \quad \rho = m/(1 + m) ,$$

(19)
where now \( t, m, z \) are related by
\[
z = t(1 + t)^4/(1 + t - t^2), \quad m = t/(1 + t - t^2),
\]
and \( t \) is small when \( z \) is. This yields the expansion
\[
\kappa = 1 + z - 2z^2 + 8z^3 - 40z^4 + 225z^5 - 1362z^6 + 8670z^7 - 57254z^8 + 388830z^9 + O(z^{10}).
\] (20)

For the honeycomb lattice, truncating \( A_i(a) \) and \( F_i(a, b) \) in (9) to one-by-one, we obtain eight distinct equations for \( \xi, \eta_1, \eta_2 \) and the elements of the matrices. We have not succeeded in significantly simplifying the solution of these eqns, but we do note that to leading order in \( z \) we can naturally choose,
\[
A_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & 0 \\ 0 & z^{1/3} \end{pmatrix},
\]
and
\[
F_1 = F_2 = \begin{pmatrix} 1 & z^{1/3} \\ z^{1/3} & z^{2/3} \end{pmatrix}.
\]
Without loss of generality we can fix \( A_1 \) to be the unit matrix, and normalise \( A_2, F_1, F_2 \) to have top-left element equal to unity. We can then iteratively solve the eight equations for the eight remaining unknowns to successively higher orders, obtaining:
\[
\kappa^2 = 1 + 2z - 2z^2 + 6z^3 - 23z^4 + 100z^5 - 469z^6 + 2314z^7 - 11841z^8 + 62286z^9 - 334804z^{10} + 1831358z^{11} - 10162680z^{12} + 57080872z^{13} + O(z^{14}).
\] (21)

We note that for each lattice this ‘Kramers-Wannier’ approximation is more accurate than the Bethe approximation, being correct for orders up to (but not including) \( z^{2q'} \).
One obtains successively more accurate approximations by taking the matrices $A, F$ to be larger. This fact is used in [6] and [7] to obtain series expansions. Here we use it to obtain accurate numerical values of $\kappa$ and $\rho$ for $z = 1$. If $A(0)$ is of size $n_0$ by $n_0$ and $A(1)$ is $n_1$ by $n_1$, then $F(0,1)$ is $n_0$ by $n_1$ and $A, F$ are $n$ by $n$, where

$$n = n_0 + n_1 .$$

From now on we re-arrange the combined matrices $A, F, S, M$ so that the entries of the diagonal matrix $A$ ($A_1 A_2$ for the honeycomb lattice) are in numerically decreasing order. Then $S$ is a diagonal matrix with entries 0 or 1, corresponding to whether the centre site is empty or full for that state. The formula (11) can still be written

$$\rho = \text{Trace } SM / \text{Trace } M .$$

5 Values of $\kappa$ and $\rho$ for $z = 1$

Throughout this section we take $z$ to be 1. For all three lattices the ‘Kramers-Wannier’ approximation has $n_0, n_1, n = 1, 1, 2$. The next approximation has $n_0, n_1, n = 2, 1, 3$. We present the numerical results obtained for the Bethe approximation and these two simple corner matrix approximations, together with those for $n_0, n_1, n = 3, 2, 5$. It is apparent that the results are converging rapidly towards a limit. For the square lattice we have continued the sequence of approximations to $n = 48$, i.e. we have kept the largest 48 diagonal elements of $A$. Then $n_0, n_1 = 29, 19$. (In fact, since writing this paper we have extended the square lattice calculation to $n = 60$, working to 55-digit accuracy, which has increased our confidence in the numerical results for this case.) Similarly for the honeycomb lattice we have continued to $n = 20$, keeping the largest 20 elements of $A_1 A_2$, with $n_0, n_1 = 11, 9$.

For the benefit of anyone who wants to repeat these calculations, in the Appendix we have given the diagonal elements of $A$ and $A_1 A_2$ for the square and honeycomb lattices with $n = 48$ and $n = 20$, respectively. In each case we have included the next-largest eigenvalue, which is obtained during the iterative solution procedure, but
not actually used in the equations (8), (9). This provides a measure of the accuracy of the approximation. The values of these elements change as one changes \( n \), but not by more than one per cent. For instance, the fifth eigenvalue of \( A \) for the square lattice occurs first when \( n = 5 \). For this and the \( n = 6, 7, 8, 48 \) truncations it is 0.0077696234, 0.0077684372, 0.0077696114, 0.0077696231, 0.0077696235. Any given element of \( A \) or \( F \) tends quite quickly to its limiting \( n = \infty \) value as \( n \) increases, once \( n \) is big enough for the element to occur at all in the truncation.

For the triangular lattice the results for \( n = 2, 3, 5 \) are given in [8]. We did not pursue the corner transfer matrix numerical calculations any further for this lattice as (a) the exact result is given in [2], in chapter 14 of [3] and (in algebraic form) in [19], (b) the fact that it is exactly solvable is connected with the fact that \( A \) has degenerate eigenvalues, at any rate in the infinite-matrix-size limit. These degeneracies actually complicate the numerical calculation, producing extra degrees of freedom that need to be fixed. Unfortunately we observed no such degeneracies for the square and honeycomb lattices, so we have no reason to suppose that they are solvable by the means used for the triangular case.

The ‘\( n = \infty \)’ results we quote for the triangular lattice are obtained from the formulae (14.1.20) and (14.5.14) of [4], using the solution of (14.1.18) to 55 significant digits:

\[
x = -0.2549635631051309947933138248965459184034888000193274011\quad (24)
\]

The solutions of (14) for the triangular, square and honeycomb lattices (with \( q = 6, 4, 3 \), respectively) are \( m = 0.2219104, 0.2755080, 0.3176722 \).

The solution of (17) is \( m = 0.1932944673 \), that of (13) is \( t = 0.3598273461 \), while for the honeycomb lattice the ‘Kramers-Wannier’ two-by-two solution of (13), (13) is \( \xi = 1.2736933548, \eta_1 = 2.4537675065, \eta_2 = 1.2413585145 \),

\[
S = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 1 & 0 \\ 0 & 0.6839628103 \end{pmatrix}
\]
Table 1: Values of $\kappa$ for the three planar lattices in the Bethe and Kramers-Wannier (KW) approximations, and using higher $n$ by $n$ corner transfer matrix truncations. The extrapolated values (exact to the accuracy given) are in the last row.

| approx. | $n$ | triangular | square | honeycomb |
|---------|-----|------------|--------|-----------|
| Bethe  | 1.42178 | 1.49365 | 1.545634 |
| KW     | 2   | 1.395217 | 1.50298407 | 1.546439299 |
|         | 3   | 1.3954858818 | 1.5030479998 | 1.546440707581 |
|         | 5   | 1.3954859724543 | 1.50304808247401 | 1.54644070878756097 |
|         | $\infty$ | 1.3954859724791398 | 1.5030480824753323 | 1.546440708787561419 |

\[
\mathcal{F}_1 = \begin{pmatrix} 1 & 0.6736226737 \\ 0.6736226737 & 0.4800087072 \end{pmatrix}, \quad \mathcal{F}_2 = \begin{pmatrix} 1 & 0.5940391501 \\ 0.5940391501 & 0.5960317063 \end{pmatrix}.
\]

The values of $\kappa$ and $\rho$ obtained are given in Tables 1 and 2, respectively. They are given to sufficient accuracy to see the convergence of the successive approximations. The deviation of an approximation from the extrapolated limit of the sequence (or what is almost the same: the deviation from the next approximation) is indeed found to be of the order of (or at most two or three orders greater than) the magnitude of the largest diagonal element of $\mathcal{M}$ omitted. This gives us some confidence that the sequence is indeed converging to the correct value, and the accuracy of the best approximation.

In fact we have obtained $\kappa$ and $\rho$ to considerably more accuracy than we are able to display in Tables 1 and 2. For the triangular, square and honeycomb lattices they are:

$\kappa = 1.3954859724793027352295006635668880689541037281446611908$ (55)  
$\kappa = 1.5030480824753322643220663294755536893857810$ (43)  
$\kappa = 1.54644070878756141848902270530472278026$ (38)
Table 2: The values of $\rho$ for the three lattices in the various approximations.

| approx. | n  | triangular          | square          | honeycomb          |
|---------|----|---------------------|-----------------|--------------------|
| Bethe   | 0.18161 | 0.215999         | 0.241086       |
| KW      | 2   | 0.161984           | 0.226281        | 0.242402036       |
|         | 3   | 0.162432600       | 0.2265703831    | 0.242407970823    |
|         | 5   | 0.162432921264    | 0.226570815452312 | 0.24240797636164382 |
|         | $\infty$ | 0.162432921397 | 0.22657081546271469 | 0.2424079763616482188 |

\[ \rho = 0.1624329213974881529255929066818976201010622684352448332 \]  \hspace{1cm} (55)

\[ = 0.22657081546271468894199226347129902640080 \]  \hspace{1cm} (41)

\[ = 0.2424079763616482188205896378263422541 \]  \hspace{1cm} (37)

The bracketted numbers are the number of decimal places given: for the triangular and square lattices we believe the results are accurate to this number of digits. For the honeycomb lattice the last two or three digits should be treated with caution.

**Next-nearest neighbour correlation**

For all these models there is of course zero probability that two adjacent sites are simultaneously occupied, i.e. $\langle \sigma_i \sigma_j \rangle = 0$ if sites $i, j$ are adjacent. For the square and honeycomb lattices, our corner transfer matrix approximations also immediately give the probability that two next-nearest-neighbour sites are simultaneously occupied. Yet higher correlations can be obtained by constructing the partition function of a small lattice, using the $A$ and $F$ matrices appropriately to include the contributions of the boundary sites and edges. For the *square* lattice, with $i, j, k, m$ being the sites shown in Fig.1, we find (to 38 decimal places)
This information is sufficient to calculate all correlations between the four sites $i, j, k, m$. Since the centre site $p$ is connected to the rest of the lattice only via $i, j, k, m$, we can use a “star-square” relation to calculate $\langle \sigma_p \rangle$ from these correlations \cite[eqn. 80]{14}, \cite[13, 15, 16]{13}. The result is the relation

$$6\rho - 4\rho_2 - 2\rho_2' + 4\rho_3 - \rho_4 = 1 \quad .$$

This is a useful check on our numerics: it is indeed satisfied to the available accuracy.

For the honeycomb lattice, with $i, j, k, m$ being the sites shown in Fig. 2, to 33 decimal places we obtain

$$\rho_2 = \langle \sigma_i \sigma_j \rangle = 0.079618322060174417313883811021777$$

$$\rho_3 = \langle \sigma_i \sigma_j \sigma_k \rangle = 0.026815084372282157838703243933620$$

$$\rho_3' = \langle \sigma_i \sigma_j \sigma_m \rangle = 0.032467404849412503526876270338554 \quad .$$

(26)
The site $p$ is connected to the rest of the lattice only via $i, j, k$, so this time we can use the “star-triangle” relation to obtain

$$5\rho - 3\rho_2 + \rho_3 = 1,$$

which is indeed satisfied to the available accuracy.

### 6 Acknowledgements

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Table 3: Diagonal elements of $A$ for the square lattice for the $n = 48$ approximation

| $i$ | $s_i$ | $a_i$  |
|-----|-------|--------|
| 1   | 0     | 1.0    |
| 2   | 1     | 0.735716 |
| 3   | 0     | 0.107349 |
| 4   | 1     | $1.65637 \times 10^{-1}$ |
| 5   | 0     | $0.776962 \times 10^{-2}$ |
| 6   | 1     | $0.100064 \times 10^{-2}$ |
| 7   | 0     | $0.737188 \times 10^{-3}$ |
| 8   | 0     | $0.260396 \times 10^{-3}$ |
| 9   | 1     | $0.772256 \times 10^{-4}$ |
| 10  | 0     | $0.593047 \times 10^{-4}$ |
| 11  | 0     | $0.133328 \times 10^{-4}$ |
| 12  | 1     | $0.108387 \times 10^{-4}$ |
| 13  | 1     | $0.582574 \times 10^{-5}$ |
| 14  | 0     | $0.504688 \times 10^{-5}$ |
| 15  | 0     | $0.195936 \times 10^{-5}$ |
| 16  | 0     | $0.879431 \times 10^{-6}$ |
| 17  | 1     | $0.696052 \times 10^{-6}$ |
| 18  | 0     | $0.423968 \times 10^{-6}$ |
| 19  | 1     | $0.360942 \times 10^{-6}$ |
| 20  | 0     | $0.110189 \times 10^{-6}$ |
| 21  | 0     | $0.707359 \times 10^{-7}$ |
| 22  | 1     | $0.604211 \times 10^{-7}$ |
| 23  | 1     | $0.427386 \times 10^{-7}$ |
| 24  | 0     | $0.372170 \times 10^{-7}$ |

Table 4: Diagonal elements of $A_1 A_2$ for the honeycomb lattice for the $n = 20$ approximation

| $i$ | $s_i$ | $a_i$  |
|-----|-------|--------|
| 11  | 1     | $1.71216 \times 10^{-9}$ |
| 12  | 0     | $6.35801 \times 10^{-10}$ |
| 13  | 1     | $6.12314 \times 10^{-10}$ |
| 14  | 0     | $9.24125 \times 10^{-11}$ |
| 15  | 0     | $1.19689 \times 10^{-11}$ |
| 16  | 1     | $1.03587 \times 10^{-11}$ |
| 17  | 1     | $4.37873 \times 10^{-12}$ |
| 18  | 0     | $3.65874 \times 10^{-12}$ |
| 19  | 0     | $8.98123 \times 10^{-13}$ |
| 20  | 1     | $1.39953 \times 10^{-13}$ |
| 21  | 0     | $6.92231 \times 10^{-14}$ |
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