

THE SHIFT OPERATOR MATRIX METHOD APPLIED TO THE TWO-DIMENSIONAL NEAREST AND NEXT NEAREST NEIGHBOR PROBLEM

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Abstract

The shift operator matrix (SOM) method is discussed. We show that in the thermodynamic limit, the largest eigenvalue of the SOM determines the grand canonical partition function for situations when simple, nearest-neighbor and next-nearest neighbor interacting particles are distributed on an $M \times N$ lattice space. In addition, we present a method for calculating the appropriate shift operator matrices.

1. Introduction

The shift operator matrix (SOM) method has its origin in the work of Fowler and Rushbrooke [1], in which they determine the occupational degeneracy for dumbbells distributed on lattice spaces of various structure and dimensionality. More recently, the SOM method has been used successfully to treat a wide range of lattice statistics problems.

The SOM method, in one form or another, has been employed to determine the occupational degeneracy for the following situations:

- (1) dumbbells on partially filled rectangular, two-dimensional lattices [2–5];
- (2) trimers on a partially filled rectangular $3 \times N$ lattice [6];
- (3) dumbbells on a partially filled rectangular three-dimensional lattice [7,8];

- (4) dumbbells on saturated rectangular two-dimensional lattices [9];
- (5) λ -bell particles on a saturated rectangular $\lambda \times N$ lattice [10];
- (6) dumbbells on partially filled triangular, hexagonal, honeycomb and Kagomé lattices [11–14];
- (7) variously-shaped particles ("tee", "ell" and trimer) on partially filled rectangular $2 \times N$ lattice spaces [15].

In addition, the SOM method has been used to obtain the composite nearest-neighbor degeneracy for simple particles [16--18] (that occupy a single site) and for interacting dumbbells [19] on a $2 \times N$ lattice.

Phares et al. have considered the problems of decoupling [20] and solving [21–23] (using combinatoric functions) the linear recursions that arise when the SOM method is employed.

The thermodynamic and statistical consequences of the SOM technique, involving the entropy, isothermal compressibility, specific heat and adsorption for rectangular lattices have also been discussed in the literature [24,25]. The SOM method has also led to an exact determination of the occupied nearest-neighbor pair density on $2 \times N$ lattices [26].

Recently, George et al. [27] have used the nearest-neighbor degeneracy, obtained by the SOM method [25], to calculate the heat capacity of submonolayer films of Ne, Ar, and Xe on graphite for several values of coverage. They obtain critical temperature values which are in very good agreement with experimental data.

As it now stands, the SOM method suffers from two deficiencies:

- (1) Even for relatively narrow lattice spaces, the effort necessary to construct the shift operator matrix is formidable.
- (2) After the SOM has been obtained, the grand canonical partition function, i.e. its largest eigenvalue, cannot be readily determined.

In some ways, the SOM method is similar to the so-called transfer matrix method [28,29]. The SOM method, however, has several advantages:

- (1) It is more straightforward to determine the elements of the matrices involved.
- (2) There is a more obvious physical/statistical interpretation of the elements of the SOM.
- (3) Given the size and dimensions of the lattice, the number of "particles" and the numbers of the various kinds of nearest-neighbor pairs, the related degeneracies can be determined explicitly.
- (4) Because the method yields an exact recursion for the basic degeneracy, all the moments of the statistics can be computed. Specifically, the dispersion for the expectation of any variable of interest can be calculated readily for finite spaces.

There is a large body of related work on this monomeric model. Although we have couched the present article in terms of vacancy/occupation of lattice sites and the associated nearest-neighbor pairs, it should be pointed out that this is equivalent to the Ising model in a magnetic field, and to the treatment of binary alloys [30–34].

In the next section, we will show that in the thermodynamic limit the grand canonical partition function (and, hence, all the thermodynamics) are contained in the largest eigenvalue of the SOM. We will also present a method by which one can readily determine the SOM for simple, interacting particles distributed on a rectangular $M \times N$ lattice.

2. The Shift Operator Matrix (SOM) method

We consider indistinguishable, simple particles (which occupy a single lattice site) distributed on a rectangular lattice space. The particles on the lattice are assumed to interact with their nearest neighbors (see double lines in fig. 1) and their next nearest neighbors (see diagonal lines in fig. 1).

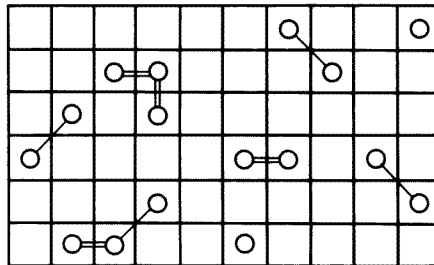


Fig. 1. In this figure, the occupied nearest-neighbor pairs are shown by a double line; the occupied next nearest neighbor by a single line. The vacant and mixed nearest- and next nearest-neighbor pairs are not shown.

To determine the composite nearest- and next-nearest neighbor degeneracy by the SOM method, we first treat a $1 \times N$ lattice and define an $\alpha_1(N)$ -space (see fig. 2) in which the site on the left-hand side, i.e. the N th site, is vacant; and an $\alpha_2(N)$ -space to be a $1 \times N$ lattice in which the N th site is occupied. (The occupation of the remaining $N - 1$ sites is not specified.) $A_1(N, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00})$ is the number of ways of arranging q particles on an $\alpha_1(N)$ -space in such a way so as to create ${}_1n_{11}$ occupied nearest-neighbor pairs, ${}_1n_{00}$ vacant nearest-neighbor pairs and ${}_2n_{11}$ occupied next nearest-neighbor pairs, as well as ${}_2n_{00}$ vacant next nearest-neighbor pairs.

Because $N - 1$ is the number of separations between sites on a $1 \times N$ lattice, it is also the total number of nearest-neighbor pairs, i.e.,

$$N - 1 = {}_1n_{11} + {}_1n_{01} + {}_1n_{00} . \tag{1}$$

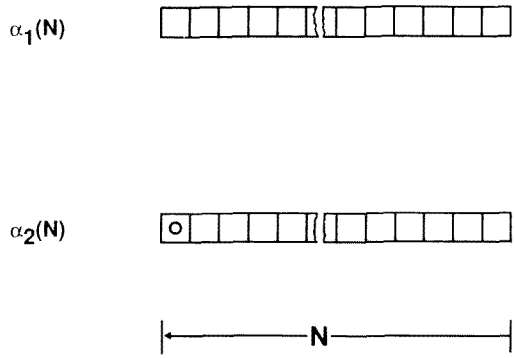


Fig. 2. These figures define the $\alpha_1(N)$ and $\alpha_2(N)$ spaces that are required for the decomposition of the composite degeneracies A_1 and A_2 . It is understood that the remaining $N - 1$ sites may or may not be occupied.

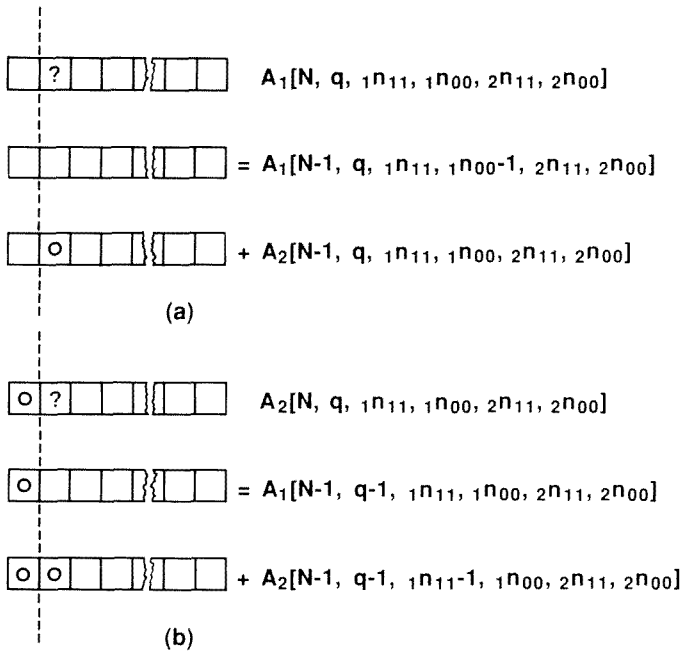


Fig. 3. This figure shows the decomposition of the composite degeneracies A_1 and A_2 .

(Here, we do not distinguish between 0-1 and 1-0 nearest-neighbor pairs.) Because next nearest-neighbor pairs are defined by the diagonal lines of fig. 1, ${}_2n_{11}$, ${}_2n_{01}$ and ${}_2n_{00}$ are assumed to be zero for a $1 \times N$ lattice.

In addition, for a $2 \times N$ lattice, $2(N - 1)$ is the total number of next nearest-neighbor pairs, i.e.,

$$2(N - 1) = {}_2n_{11} + {}_2n_{01} + {}_2n_{00} . \quad (2)$$

Thus, the argument of A_1 implies that ${}_1n_{01}$ and ${}_2n_{01}$, the numbers of mixed nearest- and next nearest-neighbor pairs are also prescribed. This can be extended for an $M \times N$ rectangular lattice to $2NM - N - M = {}_1n_{00} + {}_1n_{01} + {}_1n_{11}$ and $2NM - 2N - 2M = {}_2n_{00} + {}_2n_{01} + {}_2n_{11}$, again showing that ${}_1n_{01}$ and ${}_2n_{01}$ are prescribed once $N, M, {}_1n_{00}, {}_1n_{11}, {}_2n_{00}, {}_2n_{11}$ are given. Similarly, $A_2 [N, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}]$ is the multiplicity of arrangements for q particles on an $\alpha_2(N)$ -space, when ${}_1n_{11}, {}_1n_{00}, {}_2n_{11}$ and ${}_2n_{00}$ are prescribed.

By enquiring about the state of occupation of the $(N - 1)$ th site [see fig. 3(a)], we can write:

$$\begin{aligned} & A_1 [N, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] \\ &= A_1 [N - 1, q, {}_1n_{11}, {}_1n_{00} - 1, {}_2n_{11}, {}_2n_{00}] \\ &+ A_2 [N - 1, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] \end{aligned} \quad (3)$$

and from fig. 3(b):

$$\begin{aligned} & A_2 [N, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] \\ &= A_1 [N - 1, q - 1, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] \\ &+ A_2 [N - 1, q - 1, {}_1n_{11} - 1, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] . \end{aligned} \quad (4)$$

If we define a next nearest-neighbor pair to be along a diagonal (see fig. 1) then, in this sense, a $1 \times N$ lattice cannot have next nearest-neighbor pairs. Consequently, ${}_2n_{11}$ and ${}_2n_{00}$ are not needed in eqs. (3) and (4).

Equations (3) and (4) may be represented as

$$R \begin{pmatrix} U & 1 \\ S & ST \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \begin{pmatrix} A_1 \\ A_2 \end{pmatrix}, \quad (5)$$

where R, S, T and U are shift operators that reduce by one the quantities $N, q, {}_1n_{11}$ and ${}_1n_{00}$, respectively, i.e.,

$$\begin{aligned}
R^r S^s T^t U^u A_1 [N, q, {}_1n_{11}, {}_1n_{00}] \\
= A_1 [N - r, q - s, {}_1n_{11} - t, {}_1n_{00} - u] .
\end{aligned} \tag{6}$$

Equation (5) may be written as

$$Q_1 A = R^{-1} A , \tag{7}$$

in which

$$Q_1 \equiv \begin{pmatrix} U & 1 \\ S & ST \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} U & 1 \\ 1 & T \end{pmatrix} . \tag{8}$$

Thus, we see in eq. (8) that the matrix Q_1 , the shift operator matrix, can be decomposed into a particle matrix (in S only) and a nearest-neighbor interaction matrix (in U and T only).

As an example of the utility of the SOM method, we will use the foregoing results to obtain the grand canonical partition function for simple, indistinguishable, nearest-neighbor interacting particles distributed on a $1 \times N$ lattice space. Equation (5) may also be written

$$\begin{pmatrix} RU - 1 & R \\ RS & RST - 1 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0. \tag{9}$$

For eq. (9) to have a non-trivial solution, the determinant of the 2×2 matrix should annihilate the solution space; thus

$$[1 - RU - RST - R^2S + R^2STU] A_1 = 0, \tag{10}$$

which yields the desired recursion

$$\begin{aligned}
A_1 [N, q, n_{11}, n_{00}] &= A_1 [N - 1, q, n_{11}, n_{00} - 1] \\
&\quad + A_1 [N - 1, q - 1, n_{11} - 1, n_{00}] \\
&\quad + A_1 [N - 2, q - 1, n_{11}, n_{00}] \\
&\quad - A_1 [N - 2, q - 1, n_{11} - 1, n_{00} - 1] ,
\end{aligned} \tag{11}$$

where the pre-subscript 1 on the n 's has been dropped.

$A_2 [N, q, n_{11}, n_{00}]$ also satisfies the recursion specified by eq. (10). The only difference between A_1 and A_2 is to be found in their respective initial conditions. Because both A_1 and A_2 satisfy the same recursion, it must be a characteristic of the particle-lattice system. Thus, we conclude that A , the total degeneracy, satisfies the recursion given by equating to zero the determinant of the 2×2 matrix in eq. (9).

The initial conditions for A can be written with the understanding that $A [N, q, n_{11}, n_{00}]$ vanishes if $N < 1$ or if $q, n_{11}, n_{00} < 0$. $A [N, q, n_{11}, n_{00}]$ will also vanish if

$$q > N$$

or

$$n_{11} > q - 1$$

or

$$n_{00} > N - q - 1.$$

Then the initial conditions are

$$A [1, 0, 0, 0] = 1, \quad A [1, 1, 0, 0] = 1, \quad A [2, 0, 0, 0] = 0,$$

$$A [2, 1, 0, 0] = 2, \quad A [2, 2, 1, 0] = 1.$$

With eq. (11), we can calculate $f_{N,q}(x, y)$, the canonical partition (generating) function as

$$\begin{aligned} f_{N,q}(x, y) &\equiv \sum_{n_{11}, n_{00}} A [N, q, n_{11}, n_{00}] x^{n_{11}} y^{n_{00}} \\ &= y f_{N-1,q}(x, y) + x f_{N-1,q-1}(x, y) \\ &\quad + f_{N-2,q-1}(x, y) - x y f_{N-2,q-1}(x, y), \end{aligned} \tag{12}$$

with the initial conditions

$$f_{N,0}(x, y) = y f_{N-1,0}(x, y) \quad N \geq 2$$

$$f_{N,1}(x, y) = y f_{N-1,1}(x, y) + f_{N-2,0}(x, y) \quad N \geq 3$$

$$f_{1,0}(x, y) = 1, \quad f_{1,1}(x, y) = 1,$$

$$f_{2,1}(x, y) = 2, \quad f_{2,2}(x, y) = x. \tag{13}$$

In eqs. (12) and (13), we adopt the convention that $f_{N,q}(x, y) = 0$ if $q < 0$ or if $q > N$.

The grand canonical partition (bivariate generating) function is now written as

$$g_N(x, y, z) \equiv \sum_{q=0}^N f_{N,q}(x, y) z^q$$

$$= (y + zx)g_{N-1}(x, y, z) + z(1 - xy)g_{N-2}(x, y, z) \quad (14)$$

or

$$g_{N+2}(x, y, z) = (y + zx)g_{N+1}(x, y, z) + z[1 - xy]g_N(x, y, z), \quad (15)$$

with the initial conditions

$$g_1(x, y, z) = 1 + z \quad (16a)$$

$$g_2(x, y, z) = y + 2z + xz^2. \quad (16b)$$

To obtain an explicit relation for $g_N(x, y, z)$, we form the polynomials (super grand canonical partition function)

$$h(x, y, z, \eta) \equiv \sum_{N=1}^{\infty} g_N(x, y, z) \eta^N$$

$$= \eta \frac{r(\eta)}{s(\eta)}, \quad (17)$$

where

$$r(\eta) \equiv [1 - \eta(y + xz)]g_1 + \eta g_2$$

and

$$s(\eta) \equiv 1 - \eta(y + xz) - \eta^2 z(1 - xy).$$

We note that $r(\eta)$ depends on the initial conditions and $s(\eta)$ is the determinant of the 2×2 matrix in eq. (9), where

$$R \rightarrow \eta, \quad S \rightarrow z, \quad T \rightarrow x, \quad U \rightarrow y.$$

From

$$g_N(x, y, z) = \frac{1}{N!} \left. \frac{\partial^N h}{\partial \eta^N} \right|_{\eta=0}$$

and using the partial fraction expansion of $h(x, y, z, \eta)$, we obtain

$$g_N(x, y, z) = \sum_{j=1}^2 c_j \eta_j^{-N}, \quad (18)$$

where the c_j 's are given by

$$c_j \equiv \left. \frac{r(\eta)}{s'(\eta)} \right|_{\eta = \eta_j}, \quad (18a)$$

in which the η_j 's are the roots of the polynomial $s(\eta)$.

In the limit as $N \rightarrow \infty$

$$\ln g_N \cong -N \ln \eta_1, \quad (19)$$

where η_1 is the smallest root of $s(\eta)$.

Rearranging eq. (5), we have

$$\begin{pmatrix} U - R^{-1} & 1 \\ S & ST - R^{-1} \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = 0, \quad (20)$$

which shows that R^{-1} is an eigenvalue of the SOM. Thus, η_1^{-1} is the largest eigenvalue of Q_1 (expressed in terms of the activities x, y and z).

If one wishes to work within some other ensemble, e.g. the isothermal-isobaric ensemble [27], then $s(\eta)$ should be written as a polynomial in z , in which the coefficients of the powers of z are functions of x, y , and η .

In the foregoing discussion, we have attempted to demonstrate the utility of the SOM and its relation to the grand canonical partition function. In the remainder of the paper, therefore, we will concentrate our attention on the SOM and the manner by which its elements may be determined for two-dimensional lattices and for nearest- as well as next nearest-neighbor interacting particles.

3. Extension to $M \times N$ lattices

We first construct a $2 \times N$ lattice by uniting two $1 \times N$ lattices and initially allowing neither nearest- nor next nearest-neighbor interaction between the two rows. Then, by defining the spaces $\alpha_1(N)$, $\alpha_2(N)$, $\alpha_3(N)$ and $\alpha_4(N)$ (see fig. 4), we obtain the required relationships among the degeneracies A_1 , A_2 , A_3 and A_4 , as shown in fig. 5. These relationships may be written succinctly as

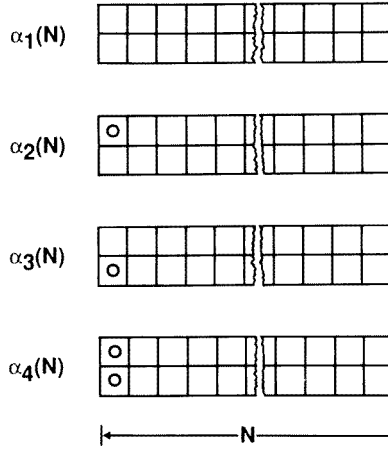


Fig. 4. These figures define $\alpha_1(N)$ -, $\alpha_2(N)$ -, $\alpha_3(N)$ - and $\alpha_4(N)$ -spaces that are needed for the decomposition of the degeneracies A_1 , A_2 , A_3 and A_4 . It is understood that the remaining $2(N - 1)$ sites may or may not be occupied.

$$\begin{pmatrix} U^2 & U & U & 1 \\ SU & STU & S & ST \\ SU & S & STU & ST \\ S^2 & S^2 T & S^2 T & S^2 T^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix} = R^{-1} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix}, \tag{21}$$

or

$$QA = R^{-1} A ,$$

where

$$Q \equiv \begin{pmatrix} U & 1 \\ S & ST \end{pmatrix} \otimes \begin{pmatrix} U & 1 \\ S & ST \end{pmatrix} = \begin{pmatrix} U & 1 \\ S & ST \end{pmatrix}^{[2]} = Q_1^{[2]}, \tag{22}$$

where \otimes implies the Kronecker product and $^{[2]}$ the Kronecker square of Q_1 .

If we now construct a $2 \times N$ lattice from two $1 \times N$ lattices and allow both nearest- and next nearest-neighbor interaction between the two rows, we obtain (see fig. 6):

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|} \hline & ? & & & & \\ \hline & ? & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & \mathbf{A}_1[\mathbf{N}, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & = \mathbf{A}_1[\mathbf{N}-1, q, {}_1n_{11}, {}_1n_{00}-3, {}_2n_{11}, {}_2n_{00}-2] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & & & & & \\ \hline & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_2[\mathbf{N}-1, q, {}_1n_{11}, {}_1n_{00}-2, {}_2n_{11}, {}_2n_{00}-1] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline \circ & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_3[\mathbf{N}-1, q, {}_1n_{11}, {}_1n_{00}-2, {}_2n_{11}, {}_1n_{00}-1] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & \circ & & & & \\ \hline \circ & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_4[\mathbf{N}-1, q, {}_1n_{11}, {}_1n_{00}-1, {}_2n_{11}, {}_2n_{00}]
 \end{array}$$

Fig. 5(a)

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & ? & & & & \\ \hline & ? & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & \mathbf{A}_2[\mathbf{N}, q, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}, {}_2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & & & & & \\ \hline & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & = \mathbf{A}_1[\mathbf{N}-1, q-1, {}_1n_{11}, {}_1n_{00}-1, {}_2n_{11}, {}_2n_{00}-1] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & \circ & & & & \\ \hline & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_2[\mathbf{N}-1, q-1, {}_1n_{11}-1, {}_1n_{00}-1, {}_2n_{11}, {}_2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & & & & & \\ \hline & \circ & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_3[\mathbf{N}-1, q-1, {}_1n_{11}, {}_1n_{00}, {}_2n_{11}-1, {}_2n_{00}-1] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & \circ & & & & \\ \hline & \circ & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_4[\mathbf{N}-1, q-1, {}_1n_{11}-1, {}_1n_{00}, {}_2n_{11}-1, {}_2n_{00}]
 \end{array}$$

Fig. 5(b)

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|} \hline & ? & & & & \\ \hline \circ & ? & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & \mathbf{A}_3[N, q, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{11}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline \circ & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & = \mathbf{A}_1[N-1, q-1, 1n_{11}, 1n_{00}-1, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & \circ & & & & \\ \hline \circ & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_2[N-1, q-1, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline \circ & \circ & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_3[N-1, q-1, 1n_{11}-1, 1n_{00}-1, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline & \circ & & & & \\ \hline \circ & \circ & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_4[N-1, q-1, 1n_{11}-1, 1n_{00}, 2n_{11}, 2n_{00}]
 \end{array}$$

Fig. 5(c)

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & ? & & & & \\ \hline \circ & ? & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & \mathbf{A}_4[N, q, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & & & & & \\ \hline \circ & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & = \mathbf{A}_1[N-1, q-2, 1n_{11}-1, 1n_{00}, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & \circ & & & & \\ \hline \circ & & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_2[N-1, q-2, 1n_{11}-2, 1n_{00}, 2n_{11}-1, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & & & & & \\ \hline \circ & \circ & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & + \mathbf{A}_3[N-1, q-2, 1n_{11}-2, 1n_{00}, 2n_{11}-1, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|} \hline \circ & \circ & & & & \\ \hline \circ & \circ & & & & \\ \hline \end{array} & \begin{array}{|c|c|c|c|c|c|} \hline & & & & & \\ \hline & & & & & \\ \hline \end{array} & = \mathbf{A}_4[N-1, q-2, 1n_{11}-3, 1n_{00}, 2n_{11}-2, 2n_{00}]
 \end{array}$$

Fig. 5(d)

Fig. 5. These figures show the decomposition of the composite next nearest-neighbor degeneracies when there is no interaction between the $1 \times N$ strips.

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & ? & & & & & & \\ \hline & ? & & & & & & \\ \hline \end{array} & = & A_1[N, q, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & & & & & & & \\ \hline & & & & & & & \\ \hline \end{array} & = & A_1[N-1, q, 1n_{11}, 1n_{00}-2, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & \circ & & & & & & \\ \hline & & & & & & & \\ \hline \end{array} & + & A_2[N-1, q, 1n_{11}, 1n_{00}-1, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & & & & & & & \\ \hline & \circ & & & & & & \\ \hline \end{array} & + & A_3[N-1, q, 1n_{11}, 1n_{00}-1, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & \circ & & & & & & \\ \hline & \circ & & & & & & \\ \hline \end{array} & + & A_4[N-1, q, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{00}]
 \end{array}$$

Fig. 6(a)

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & ? & & & & & & \\ \hline & ? & & & & & & \\ \hline \end{array} & = & A_2[N, q, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & & & & & & & \\ \hline & & & & & & & \\ \hline \end{array} & = & A_1[N-1, q-1, 1n_{11}, 1n_{00}-1, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & \circ & & & & & & \\ \hline & & & & & & & \\ \hline \end{array} & + & A_2[N-1, q-1, 1n_{11}-1, 1n_{00}-1, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & & & & & & & \\ \hline & \circ & & & & & & \\ \hline \end{array} & + & A_3[N-1, q-1, 1n_{11}, 1n_{00}, 2n_{11}, 2n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & \circ & & & & & & \\ \hline & \circ & & & & & & \\ \hline \end{array} & + & A_4[N-1, q-1, 1n_{11}-1, 1n_{00}, 2n_{11}, 2n_{00}]
 \end{array}$$

Fig. 6(b)

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & ? & & & & & & \\ \hline \circ & ? & & & & & & \\ \hline \end{array} & \mathbf{A}_3[\mathbf{N}, \mathbf{q}, \mathbf{1}n_{11}, \mathbf{1}n_{00}, \mathbf{2}n_{11}, \mathbf{2}n_{11}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & & & & & & & \\ \hline \circ & & & & & & & \\ \hline \end{array} & = \mathbf{A}_1[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{1}, \mathbf{1}n_{11}, \mathbf{1}n_{00}-\mathbf{1}, \mathbf{2}n_{11}, \mathbf{2}n_{00}-\mathbf{1}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & \circ & & & & & & \\ \hline \circ & & & & & & & \\ \hline \end{array} & + \mathbf{A}_2[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{1}, \mathbf{1}n_{11}, \mathbf{1}n_{00}, \mathbf{2}n_{11}-\mathbf{1}, \mathbf{2}n_{00}-\mathbf{1}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & & & & & & & \\ \hline \circ & \circ & & & & & & \\ \hline \end{array} & + \mathbf{A}_3[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{1}, \mathbf{1}n_{11}-\mathbf{1}, \mathbf{1}n_{00}-\mathbf{1}, \mathbf{2}n_{11}, \mathbf{2}n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline & \circ & & & & & & \\ \hline \circ & \circ & & & & & & \\ \hline \end{array} & + \mathbf{A}_4[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{1}, \mathbf{1}n_{11}-\mathbf{1}, \mathbf{1}n_{00}, \mathbf{2}n_{11}-\mathbf{1}, \mathbf{2}n_{00}]
 \end{array}$$

Fig. 6(c)

$$\begin{array}{l}
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & ? & & & & & & \\ \hline \circ & ? & & & & & & \\ \hline \end{array} & \mathbf{A}_4[\mathbf{N}, \mathbf{q}, \mathbf{1}n_{11}, \mathbf{1}n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & & & & & & & \\ \hline \circ & & & & & & & \\ \hline \end{array} & = \mathbf{A}_1[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{2}, \mathbf{1}n_{11}, \mathbf{1}n_{00}, \mathbf{2}n_{11}, \mathbf{2}n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & \circ & & & & & & \\ \hline \circ & & & & & & & \\ \hline \end{array} & + \mathbf{A}_2[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{2}, \mathbf{1}n_{11}-\mathbf{1}, \mathbf{1}n_{00}, \mathbf{2}n_{11}, \mathbf{2}n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & & & & & & & \\ \hline \circ & \circ & & & & & & \\ \hline \end{array} & + \mathbf{A}_3[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{2}, \mathbf{1}n_{11}-\mathbf{1}, \mathbf{1}n_{00}, \mathbf{2}n_{11}, \mathbf{2}n_{00}] \\
 \\
 \begin{array}{|c|c|c|c|c|c|c|c|} \hline \circ & \circ & & & & & & \\ \hline \circ & \circ & & & & & & \\ \hline \end{array} & = \mathbf{A}_4[\mathbf{N}-\mathbf{1}, \mathbf{q}-\mathbf{2}, \mathbf{1}n_{11}-\mathbf{2}, \mathbf{1}n_{00}, \mathbf{2}n_{11}, \mathbf{2}n_{00}]
 \end{array}$$

Fig. 6(d)

Fig. 6. These figures show the decomposition of the composite next nearest-neighbor degeneracies when nearest- and next nearest-neighbor interaction occurs between the $1 \times N$ strips.

$$\begin{pmatrix} U^3W^2 & U^2W & U^2W & U \\ SUW & STU & SVW & STV \\ SUW & SVW & STU & STV \\ S^2T & S^2T^2V & S^2T^2V & S^2T^3V^2 \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix} = R^{-1} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix}, \quad (23)$$

where V and W are the shift operators associated with ${}_2n_{11}$ and ${}_2n_{00}$, respectively. Equation (23) may be written as

$$Q_2 A = R^{-1} A, \quad (24)$$

where

$$Q_2 = \begin{pmatrix} U^3W^2 & U^2W & U^2W & U \\ SUW & STU & SVW & STV \\ SUW & SVW & STU & STV \\ S^2T & S^2T^2V & S^2T^2V & S^2T^3V^2 \end{pmatrix}. \quad (25)$$

Q_2 may be written as the Hadamard product of two matrices, i.e.,

$$Q_2 = P_2 \odot Q_1^{[2]}, \quad (26)$$

where

$$P_2 = \begin{pmatrix} UW^2 & UW & UW & U \\ W & 1 & VW & V \\ W & VW & 1 & V \\ T & TV & TV & TV^2 \end{pmatrix}, \quad (27)$$

in which P_2 can also be decomposed into the Hadamard product of two matrices, one of which depends on nearest-neighbor shift operators and the other on next nearest-neighbor shift operators, i.e.,

$$P_2 = {}_1P_2 \odot {}_2P_2, \quad (28)$$

where

$${}_1P_2 \equiv \begin{pmatrix} U & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & T \end{pmatrix} \quad (29)$$

and where ${}_2P_2$

$${}_2P_2 \equiv \begin{pmatrix} W^2 & W & W & 1 \\ W & 1 & WV & V \\ W & WV & 1 & V \\ 1 & V & V & V^2 \end{pmatrix}. \quad (30)$$

That is, ${}_1P_2$ describes the nearest-neighbor interaction between particles in one $1 \times N$ lattice with particles in the other $1 \times N$ lattice. Similarly, ${}_2P_2$ describes the *next* nearest-neighbor interaction between particles of one row with the other.

If we continue the process by "adding" a $1 \times N$ lattice to a $2 \times N$ lattice to create a $3 \times N$ lattice, we obtain [by analogy with eq. (24)]:

$$Q_3 A = R^{-1} A, \quad (31)$$

where

$$Q_3 \equiv P'_3 \odot Q_1 \otimes Q_2, \quad (32)$$

in which the matrix P'_3 is given by

$$P'_3 \equiv \begin{pmatrix} UW^2 & UW^2 & UW & UW & UW & UW & U & U \\ UW^2 & UW^2 & UW & UW & UW & UW & U & U \\ W & W & 1 & 1 & VW & VW & V & V \\ W & W & 1 & 1 & VW & VW & V & V \\ W & W & VW & VW & 1 & 1 & V & V \\ W & W & VW & VW & 1 & 1 & V & V \\ T & T & TV & TV & TV & TV & TV^2 & TV^2 \\ T & T & TV & TV & TV & TV & TV^2 & TV^2 \end{pmatrix}. \quad (33)$$

Although P'_3 may be decomposed [in analogy with eq. (28)] into the Hadamard product of two matrices, one of which depends on T and U only and the other on V

and W only, we will not do so as it is not germane to the following development. We observe only that

$$P'_3 = P_2 \otimes J_2, \tag{34}$$

where $J_2 \equiv \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ (see, for example, ref. [35]).

Thus, eq. (32) may be written

$$\begin{aligned} Q_3 &= [P_2 \otimes J_2] \odot \{Q_1 \otimes [P_2 \odot (Q_1 \otimes Q_1)]\} \\ &= [P_2 \otimes J_2] \odot \{Q_1 \otimes [P_2 \odot Q_1^{[2]}]\} \\ &= [P_2 \otimes J_2] \odot \{[J_2 \odot Q_1] \otimes [P_2 \odot Q_1^{[2]}]\} \\ &= [P_2 \otimes J_2] \odot [J_2 \otimes P_2] \odot Q_1^{[3]}, \end{aligned} \tag{35}$$

where we have used the fact that when V_1 and V_3 as well as V_2 and V_4 are the same order

$$(V_1 \otimes V_2) \odot (V_3 \otimes V_4) = (V_1 \odot V_3) \otimes (V_2 \odot V_4), \tag{36}$$

(the mixed product rule).

Equation (35) may be written

$$Q_3 = P_3 \odot Q_1^{[3]}, \tag{37}$$

where

$$P_3 \equiv [P_2 \otimes J_2] \odot [J_2 \otimes P_2]. \tag{38}$$

To make the generalization manifest, we consider a $4 \times N$ lattice:

$$Q_4 A = R^{-1} A, \tag{39}$$

where we combine a $1 \times N$ lattice with a $3 \times N$ lattice

$$\begin{aligned} Q_4 &= P'_4 \odot Q_1 \otimes Q_3 \\ &= [P_2 \otimes J_2^{[2]}] \odot [Q_1 \otimes Q_3] \\ &= [P_2 \otimes J_2^{[2]}] \odot \{Q_1 \otimes [P_3 \odot Q_1^{[3]}]\} \end{aligned}$$

$$\begin{aligned}
&= [P_2 \otimes J_2^{[2]}] \odot \{Q_1 \otimes [(P_2 \otimes J_2) \odot (J_2 \otimes P_2) \odot Q_1^{[3]}]\} \\
&= [P_2 \otimes J_2^{[2]}] \odot \{[J_2 \odot Q_1] \otimes [[P_2 \otimes J_2] \odot [J_2 \otimes P_2] \odot Q_1^{[3]}]\} \\
&= [P_2 \otimes J_2^{[2]}] \odot \{J_2 \otimes [(P_2 \otimes J_2) \odot (J_2 \otimes P_2)] \odot Q_1^{[4]}\} \\
&= [P_2 \otimes J_2^{[2]}] \odot \{[J_2 \odot J_2] \otimes [P_2 \otimes J_2] \odot [J_2 \otimes P_2] \odot Q_1^{[4]}\} \\
&= [P_2 \otimes J_2 \otimes J_2] \odot [J_2 \otimes P_2 \otimes J_2] \odot [J_2 \otimes J_2 \otimes P_2] \odot Q_1^{[4]} \\
&= P_4 \odot Q_1^{[4]}, \tag{40}
\end{aligned}$$

where

$$P_4 = \prod_{\odot, i=1}^3 \prod_{\otimes, j=1}^3 \alpha_{ij}, \tag{41}$$

in which \prod_{\odot} denotes the Hadamard product and \prod_{\otimes} the Kronecker product, and where

$$\alpha_{ij} \equiv \begin{cases} P_2 & i = j \\ J_2 & i \neq j \end{cases}.$$

Thus, for an $M \times N$ space, one may write by analogy with eqs. (25), (37) and (38), (40) and (41)

$$Q_M A = R^{-1} A, \tag{42}$$

where

$$Q_M \equiv P_M \odot Q_1^{[M]}, \tag{43}$$

in which

$$P_M \equiv \prod_{\odot, j=1}^{M-1} \prod_{\otimes, i=1}^{M-1} \alpha_{ij}, \tag{44}$$

where

$$\alpha_{ij} \equiv \begin{cases} P_2 & i = j \\ J_2 & i \neq j \end{cases}. \tag{45}$$

Thus, Q_M may be considered as the Hadamard product of two matrices, one of which, $Q_1^{[M]}$, is the matrix describing the M non-interacting $1 \times N$ strips and the other, P_M , describes both the nearest- and next nearest-neighbor interaction of one $1 \times N$ strip with its neighbor(s).

It should be noted that when the next nearest-neighbor interaction is turned off, i.e. when $W = V = 1$, eqs. (42), (43), (44) and (45) reduce to the equations appropriate to the nearest-neighbor case.

4. Conclusions

The utility of the SOM method to treat two-dimension lattice statistics problems has been discussed. The SOM has been determined for a system of simple, nearest- and next nearest-neighbor interacting particles distributed on an $M \times N$ lattice space.

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