MIXED NEAREST NEIGHBOR DEGENERACY FOR PARTICLES ON A ONE-DIMENSIONAL LATTICE SPACE

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1. INTRODUCTION

In a recent article [1] expressions were presented which describe exactly the number of independent ways of arranging q indistinguishable particles on a one-dimensional lattice space of N equivalent compartments, in such a way as to create

1. n_{11} occupied nearest neighbor pairs
2. n_{00} vacant nearest neighbor pairs.

The present paper is concerned with the degeneracy associated with n_{01}, the number of mixed (one compartment empty, one occupied) nearest neighbor pairs.

Ising [2] has developed relationships which describe approximately the degeneracy associated with mixed nearest neighbor pairs. The purpose of the present paper is to develop an expression which describes exactly the degeneracy of arrangements containing a prescribed number of mixed nearest neighbor pairs.

2. CALCULATION

To determine $A(n_{01}, q, N)$, the number of independent arrangements arising when q particles are placed on a one-dimensional lattice space of N equivalent compartments in such a way as to create n_{01} mixed nearest neighfor pairs, we must consider the situations when n_{01} is odd and when it is even.

1. n_{01} odd

When n_{01} is odd, one and only one end compartment must be occupied. (See Fig. 1.) If the occupied end compartment is on the left-hand side we construct "units" consisting of a particle or of a continguous group of particles *and* the adjacent vacancy just to the right then we observe that there are $\dfrac{n_{01}-1}{2}$ permutable "units." We initially regard these "units" as identical regardless of the number of particles ($\geqslant 1$) of which they are composed (see cross-hatched "units" in Fig. 1). These "units" can be permuted to form other independent arrangements having the same n_{01}.

There are $N - q$ vacancies but not all of these vacancies can be permuted to form independent arrangements; there are $\dfrac{n_0 - 1}{2} + 1$ vacancies which form mixed nearest neighbor pairs. Thus there are $N - q - \left(\dfrac{n_0-1}{2}\right) - 1$ permutable vacancies and a total of $N - q - 1$ objects which can be permuted. These can be arranged in

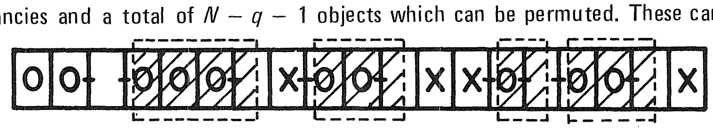

Figure 1. Shown is an arrangement of $q = 10$ particles on a linear array of $N = 19$ equivalent compartments which creates $n_{01} = 9$ mixed nearest neighbor pairs. There are $\left(\dfrac{n_{01}-1}{2}\right) = 4$ permutable "units" (cross-hatched) and $N - q - 1 - \left(\dfrac{n_{01}-1}{2}\right) = 4$ permutable vacancies (marked with x's). Thus there are a total of eight objects to be permuted while still keeping the left-hand compartment occupied.

$$\binom{N-q-1}{\frac{n_{01}-1}{2}} = \binom{N-q-1}{n-q-1\left(\frac{n_{01}-1}{2}\right)}$$

ways.

The "units" are, of course, not identical; the particles may be arranged to form "units" consisting of various numbers of particles subject to the constraint that n_{01} mixed nearest neighbor pairs must be present. To determine the number of ways the q particles can be arranged to form the $\left(\frac{n_{01}-1}{2}\right)$ "units" we consider $q-1$ lines which symbolize the separation of the q particles. (See Fig. 2.) $\left(\frac{n_{01}-1}{2}\right)$ of these lines symbolize the separation of the particles by two mixed nearest neighbor pairs and $q-1-\left(\frac{n_{01}-1}{2}\right)$ lines symbolize the adjacency of two particles. These $q-1$ lines, of which $\left(\frac{n_{01}-1}{2}\right)$ are one kInd and the remainder another kind can be arranged in $\binom{q-1}{\frac{n_{01}-1}{2}}$ ways.

Thus, if we require that the compartment on the left end of the array is occupied (and the end compartment on the right is empty) then there are

$$\binom{N-q-1}{\frac{n_{01}-1}{2}}\binom{q-1}{\frac{n_{01}-1}{2}}$$

independent arrangement possible. Of course the end compartment on the right could have been occupied (and the end compartment on the left empty) so that if n_{01} is odd we obtain

$$A(n_{01}, q, N) = 2\binom{N-q-1}{\frac{n_{01}-1}{2}}\binom{q-1}{\frac{n_{01}-1}{2}} \tag{1}$$

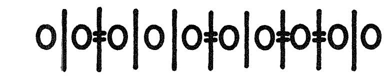

Figure 2. Figure 2 considers the particular arrangement shown in Fig. 1. There are $q-1=9$ separations between 10 particles. Of these separations $\left(\frac{n_{01}-1}{2}\right)=4$ are separations which constitute two mixed nearest neighbor pairs (two short horizontal lines) and $q-1-\left(\frac{n_{01}-1}{2}\right)=5$ represent separations between occupied nearest neighbor pairs. The q separations may be arranged in $\binom{9}{5}=126$ independent ways.

2. n_{01} even

When n_{01} is even two situations can arise:

(a) the compartments on each end of the array are empty (see Fig. 3)

(b) both end compartments are occupied (see Fig. 4).

For arrangements consistent with situation (a) there are always $\left(\frac{n_{01}}{2}\right)$ "units," each of which consists of a particle or a contiguous group of particles together with a facancy (if one is needed) to separate a "unit" from other "units," i.e., to create a mixed nearest neighbor pair. As before we initially regard these "units" as identical regardless of their composition. There are $N-q$ vacancies but not all of them are permutable; $\frac{n_{01}-2}{2}$ of

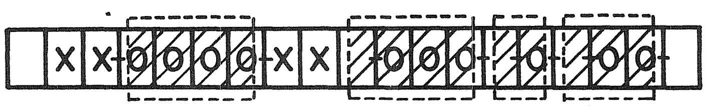

Figure 3. In this figure $N = 19$, $q = 10$, $n_{01} = 8$ and both end compartments are empty. There are $\left(\frac{n_{01}}{2}\right)$ "units" (cross-hatched) and $N - q - 1 - \left(\frac{n_{01}}{2}\right) = 4$ permutable vacancies (marked with x's) or a total of 8 objects which can be permited in $\binom{8}{4}$ ways to form independent arrangements.

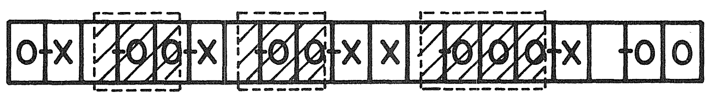

Figure 4. In this figure $N = 19$, $q = 10$, $n_{01} = 8$ and both end compartments are occupied. There are $\left(\frac{n_{01}-2}{2}\right) = 3$ permutable "units" (cross-hatched) and $N - q - 1 - \left(\frac{n_{01}-2}{2}\right) = 5$ permutable vacancies (marked with x's) or a total of 8 objects which can be permited in $\binom{8}{3}$ ways.

these vacancies are required to form mixed nearest neighbor pairs because one of the "units" (either the one to the extreme right or to the extreme left of the array) does not need a vacancy to isolate it. In addition, two vacancies, one at each end, are not permutable. Thus there are

$$N - q - \left(\frac{n_{01}}{2} - 1\right) - 2 = N - q - 1 - \frac{n_{01}}{2}$$

permutable vacancies and a total of

$$N - q - 1 - \frac{n_{01}}{2} + \frac{n_{01}}{2} = N - q - 1$$

permutable objects. These can be arranged in

$$\begin{pmatrix} N-q-1 \\ \frac{n_{01}}{2} \end{pmatrix} = \begin{pmatrix} N-q-1 \\ N-q-1-\frac{n_{01}}{2} \end{pmatrix}$$

independent ways.

The "units" are not identical as we have assumed. There are

$$\begin{pmatrix} q-1 \\ \frac{n_{01}}{2} - 1 \end{pmatrix}$$

ways of arranging the q particles in the $\left(\frac{n_{01}}{2}\right)$ "units." This can be shown by the following reasoning. There are $q - 1$ lines that symbolize the separation of the q particles (see Fig. 5). Of these lines

$$\left(\frac{n_{01}-2}{2}\right)$$

represent separations of the particles by two mixed nearest neighbor pairs and

$$q - 1 - \left(\frac{n_{01}-2}{2}\right)$$

lines symbolize the separation of adjacent particles. These $q - 1$ lines can thus be arranged in

$$\begin{pmatrix} q-1 \\ \frac{n_{01}-2}{2} \end{pmatrix}$$

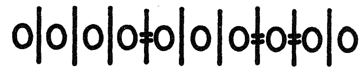

Figure 5. This figure considers the particular arrangement shown in Fig. 3. There are $q - 1 = 9$ separations between $q = 10$ particles. Of these separations $\left(\frac{n_{01}}{2}\right) - 1 = 3$ form two mixed neighbor pairs (short double horizontal lines) and

$$q - 1 - \left(\frac{n_{01}}{2} - 1\right) = 6$$

are occupied nearest neighbor pairs. The 9 separations may be arranged in $\binom{9}{6}$ independent ways. Thus the particles may be arranged within the $\frac{n_{01}}{2} = 4$ "units" in 21 ways so that there is at least one particle per unit.

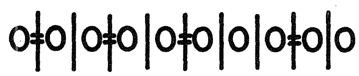

Figure 6. This figure considers the particular arrangement shown in Fig. 4. There are $q - 1 = 9$ separations between the $q = 10$ particles. Of these separations $\left(\frac{n_{01}}{2}\right) = 4$ represent separations by two mixed nearest neighbor pairs and $9 - 4 = 5$ represent separations of occupied nearest neighbor pairs. These 9 separations may be arranged in $\binom{9}{5}$ ways.

ways. This is the number of ways the q particles can be arranged to form $\left(\frac{n_{01}}{2}\right)$ "units" when the compartments on both ends are vacant.

Thus when both end compartments are empty there are

$$\binom{N - q - 1}{\frac{n_{01}}{2}}\binom{q - 1}{\frac{n_{01}}{2} - 1}$$

ways of arranging the q particles to yield exactly n_{01} nearest neighbor pairs.

For situation (b) there are $\left(\frac{n_{01} - 2}{2}\right)$ permutable "units" composed of a particle or group of contiguous particles and a vacancy to separate the "unit" for other "units." (See Fig. 4.) There are $N - q - 1 - \left(\frac{n_{01} - 2}{2}\right)$ permutable vacancies or a total of $N - q - 1$ objects which can be permuted. These objects can be arranged in

$$\binom{N - q - 1}{\frac{n_{01} - 2}{2}}$$

ways. Within the $\left(\frac{n_{01}}{2}\right)$ "units" the particles can be arranged in

$$\binom{q - 1}{\frac{n_{01}}{2}}$$

ways. This arises because there are $q - 1$ lines symbolizing the separation of the q particles (see Fig. 6); of these lines $\frac{n_{01}}{2}$ constitute separations of the "units" by two mixed nearest neighbor pairs and $q - 1 - \frac{n_{01}}{2}$ are lines which separate adjacent particles. These $q - 1$ lines can thus be arranged

$$\binom{q-1}{\frac{n_{01}}{2}}$$

ways.

Consequently, when both end compartments are occupied the q particles may be arranged in

$$\binom{N-q-1}{\frac{n_{01}}{2}-1}\binom{q-1}{\frac{n_{01}}{2}}$$

ways.

Thus the total number of arrangements possible when n_{01} is even is

$$A(n_{01}, q, N) = \binom{N-q-1}{\frac{n_{01}}{2}}\binom{q-1}{\frac{n_{01}}{2}-1} + \binom{N-q-1}{\frac{n_{01}}{2}-1}\binom{q-1}{\frac{n_{01}}{2}} \tag{2}$$

$$= 2\left(\frac{N-n_{01}}{n_{01}}\right)\binom{N-q-1}{\frac{n_{01}}{2}-1}\binom{q-1}{\frac{n_{01}}{2}-1}$$

Normalization for $A(n_{01}, q, N)$ can be shown to be

$$\sum_{n_{01}} A(n_{01}, q, N) = \binom{N}{q} \tag{3}$$

where $A(n_{01}, q, N)$ is given alternately by Eq. 1 and 2 and where the sum is over all possible values of n_{01}.

REFERENCES

1. R. B. McQuistan, *Jour. Math. Phys.,* 13, 1317 (1972).
2. E. Ising, *Z. Physik,* 31, 253 (1925).

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