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THE OCCUPATIONAL DEGENERACY FOR λ-BELL PARTICLES ON A SATURATED $\lambda \times N$ LATTICE SPACE*

J. L. HOCK
Marquette University, Milwaukee, WI 53233

and

R. B. McQUISTAN
University of Wisconsin-Milwaukee, Milwaukee, WI 53201

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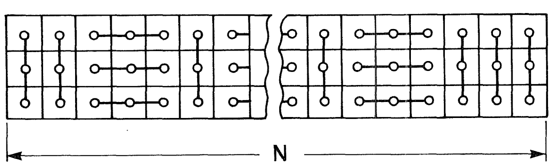
1. INTRODUCTION

A number of physical phenomena, e.g., adsorption, crystallization, magnetism, can be treated by considering the occupation statistics of lattice spaces. One of the interesting problems that arise from such an approach is that of determining the occupational degeneracy of λ-bell particles on lattice spaces of various dimensionalities. Exact solutions for one-dimensional spaces have been found for dumbbells [1, 2] ($\lambda = 2$) and for λ-bell particles [3] but exact solutions for spaces of higher-order dimensionality have only been obtained for dumbbells for very special cases [4, 5]. Consequently, approximation methods [6-8] have been used to attack this problem.

The present paper is concerned with a determination of the occupational degeneracy for indistinguishable λ-bell particles that completely fill a $\lambda \times N$ rectangular lattice space (see Fig. 1).



This figure shows one arrangement for $\lambda = 3$ particles that fill completely a $3 \times N$ lattice space.

FIGURE 1

We first derive a recursion relationship that describes exactly the multiplicity of arrangements when the $\lambda \times N$ lattice space is saturated.

In Sections 3 and 4, we derive an exact summation representation for the degeneracy and present the corresponding generating functions and continuous representation for large values of N.

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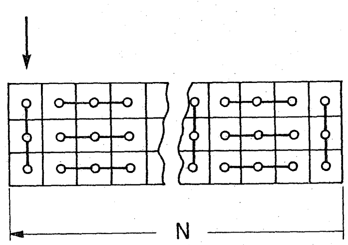
2. EXACT RECURSION RELATIONSHIP

Consider A_N to be the set of all possible arrangements of indistinguishable λ-bell particles on a completely filled $\lambda \times N$ lattice space. A_N can be considered to consist of two subsets, each of which is characterized by the state of occupation of the column of sites at one end of the space. One subset is identified by the occupation of the end column by a single (vertical) λ-bell particle (see Fig. 2a). In such a case, the remaining $(N - 1)$ λ-bell particles can be arranged on the remaining $\lambda \times (N - 1)$ lattice sites in A_{N-1} independent ways. The other subset of which A_N is composed consists of those arrangements in which the λ sites of the end column are occupied by λ (horizontal) λ-bell particles (see Fig. 2b). The remaining $(N - \lambda)$ λ-bell particles can be arranged in $A_{N-\lambda}$ independent ways. Thus

$$A_N = A_{N-1} + A_{N-\lambda} \qquad (\lambda > 1) \tag{1}$$

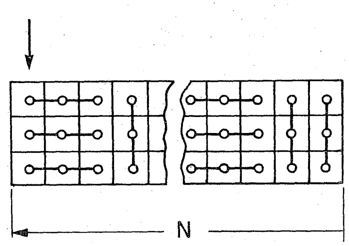
If $\lambda = 2$, Eq. 1 becomes the Fibonacci recursion [9] and

$$A_N = \frac{1}{2^{N+1}\sqrt{5}}\{[1 + \sqrt{5}]^{N+1} - [1 - \sqrt{5}]^{N+1}\}. \tag{2}$$



(a)

This arrangement is one member of the subset of A_N that is characterized by the fact that all the compartments of the column at the left-hand end are occupied by a single, vertical $\lambda = 3$ particle.



(b)

This arrangement is one member of the subset of A_N that is characterized by the fact that each compartment of the column on the left-hand end of the lattice space is occupied by three different $\lambda = 3$ particles.

FIGURE 2

For recursion relations of the kind given in Eq. 1, we may write [9]

$$A_N = C(R)^N \tag{3}$$

where C and R are not functions of N but depend on λ. Substituting Eq. 3 into Eq. 1 yields

$$R^{\lambda} - R^{\lambda-1} - 1 = 0 \tag{4}$$

or

$$T^{\lambda} + T - 1 = 0 \tag{5}$$

where $T \equiv R^{-1}$.

If λ is even, then by Descartes' rule of signs, we see that there are two real roots, one greater than unity and one less than unity; and $\left[\frac{\lambda - 2}{2}\right]$ pairs of complex roots, the largest absolute value of which is less than the largest real root. If λ is odd, then there is one real root whose value is greater than the absolute value of any of the $\left[\frac{\lambda - 1}{2}\right]$ pairs of complex roots. Thus, for large values of N,

$$A_N = C(R_1)^N \tag{6}$$

where R_1 is the largest (real) root of Eq. 4.

Figure 3 shows $R_1^{-1} = T_1$ as a function of λ. Note that T_1 approaches unity for large values of λ.

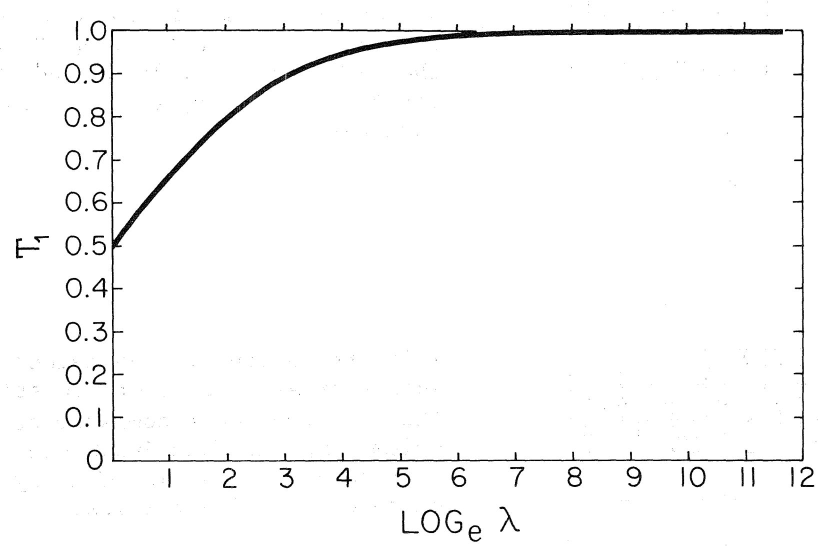


FIGURE 3. T_1 THE SMALLEST ROOT OF EQUATION 5 AS A FUNCTION OF λ

In Section 4, we will calculate the bivariant generating function which can be utilized to determine numerical values for C.

3. SUMMATION REPRESENTATION

Another representation of the occupational degeneracy can be developed through the following considerations. There are essentially two kinds of entities on the lattice space under consideration: vertical particles and groups of horizontal particles (each group consists of a block of λ particles) (see Fig. 4). If there are $q_h' = q_h/\lambda$ groups of horizontal particles (where each group occupies λ columns and λ rows), then there are $N - \lambda q_h'$ vertical particles. Thus, there are a total of

$$q_h' + N - \lambda q_h' = N - q_h'(\lambda - 1)$$

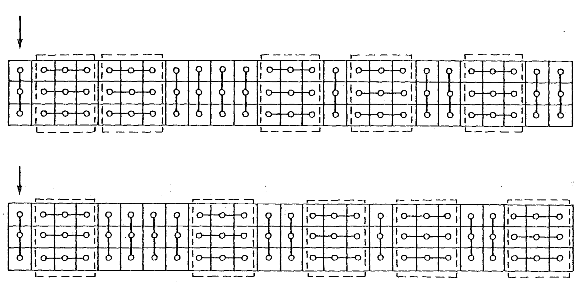
different individuals of which q_h' are one kind (the blocks of horizontal particles) and $N - \lambda q_h'$ are another (the vertical particles). These may be permuted in

$$\binom{N - q_h'(\lambda - 1)}{q_h'}$$

independent ways [3]. Thus, the total degeneracy is obtained by summing over all values of q_h',

$$A_N = \sum_{q_h'=0}^{[N/\lambda]} \binom{N - q_h'(\lambda - 1)}{q_h'}, \tag{7}$$

where $[N/\lambda]$ is the largest integer contained in N/λ.



This figure shows, for $\lambda = 3$ particles, two arrangements out of a total of $\binom{15}{5} = \binom{15}{10}$ arrangements that are possible when ten vertical particles and fifteen horizontal particles [which must be arranged in five groups] are distributed on a 3×25 lattice space.

FIGURE 4

4. GENERATING FUNCTIONS

According to Eq. 7, we form the polynomials [10]

$$u_N(x) = \sum_{k=0}^{[N/\lambda]} \binom{N - k(\lambda - 1)}{k} x^k; \tag{8}$$

then, utilizing Eq. 1, we see that

$$u_N(x) = u_{N-1}(x) + xu_{N-\lambda}(x), \tag{9}$$

with the initial conditions

$$u_0(x) = u_1(x) = \cdots = u_{\lambda-1}(x) = 1, \tag{10}$$

which reflect the fact that, if $N \leqslant \lambda - 1$, there is only one way in which the space can be completely filled; i.e., all the particles must be vertical.

The so-called bivariant generating function can be obtained as follows:

$$\begin{aligned} u(x, y) &= \sum_{N=0}^{\infty} u_N(x)y^N \\ &= \left[\frac{y^\lambda - 1}{-1}\right] + y\left\{u(x, y) - \frac{y^{\lambda-1} - 1}{y - 1}\right\} + xy^\lambda u(x, y) \end{aligned} \tag{11}$$

or

$$u(x, y) = [1 - y - xy^\lambda]^{-1}. \tag{12}$$

On the basis of Eq. 12, we may write

$$\begin{aligned} u(1, y) &= [1 - y - y^\lambda]^{-1} \\ &= \sum_{N=0}^{\infty} u_N(1)y^N \\ &= \sum_{N=0}^{\infty} A_N y^N. \end{aligned} \tag{13}$$

But, by partial fraction expansion,

$$\frac{1}{1 - y - y^\lambda} = \sum_{j=1}^{\lambda} \frac{C_j}{1 - S_j y} = \sum_{j=1}^{\lambda} \sum_{\ell=0}^{\infty} C_j [S_j y]^\ell, \tag{14}$$

where the C_j's are constants (not functions of N), and S_j are the reciprocals of the roots of $1 - y - y^\lambda$; i.e., S_j are the roots of Eq. 4. Thus, $S_j \equiv R_j$. By comparing Eqs. 13 and 14, we obtain

$$A_N = \sum_{j=1}^{\lambda} C_j [R_j]^N. \tag{15}$$

To determine the C_j's, we let $y \to R_j^{-1}$, then the dominant term in the partial fraction expansion, Eq. 14, is $\dfrac{C_j}{1 - R_j y}$. We may then write

$$\lim_{y \to R_j^{-1}} \left\{\frac{1}{1 - y - y^\lambda} - \frac{C_j}{1 - R_j y}\right\} = 0. \tag{16}$$

Applying L'Hôpital's rule yields

$$C_j = \lim_{y \to R_j^{-1}} \left[\frac{1 - R_j y}{1 - y - y^\lambda}\right] = \lim_{y \to R_j^{-1}} \left[\frac{R_j}{1 + \lambda y^{\lambda-1}}\right] = \frac{R_j}{1 + \lambda R_j^{1-\lambda}}, \tag{17}$$

and Eq. 15 becomes

$$A_N = \sum_{j=1}^{\lambda} \frac{R_j}{1 + \lambda R_j^{1-\lambda}} R_j^N \tag{18}$$

If R_1 is the dominant root, then as $N \to \infty$,

$$A_N = \frac{R_1^{N+1}}{1 + \lambda R_1^{1-\lambda}} = \frac{R_1}{1 + \lambda R_1^{1-\lambda}} R_1^N \tag{19}$$

so that the C in Eq. 6 is given by

$$C = \frac{R_1}{1 + \lambda R_1^{1-\lambda}}. \tag{20}$$

As an example, for $\lambda = 3$, $R_1 = 1.46557123$ and $C = 0.611491992$, so that

$$A_N = 0.611491992(1.46557123)^N \tag{21}$$

For $N = 10$, Eq. 21 yields a value of 27.96. This is compared to an actual value of 28 or an error of 0.14%.

Note that as λ becomes large, $C \to R_1$, so that (see Eq. 6)

$$A_N = R_1^{N+1} \quad \text{(for large values of } N \text{ and } \lambda). \tag{22}$$

CONCLUSION

The occupational degeneracy for a $\lambda \times N$ lattice space completely covered with λ-bell particles can be represented exactly by a two-term recursion relationship and by the summation of certain binomial coefficients. The appropriate generating functions have been derived and utilized to develop a continuous representation for the degeneracy as $N \to \infty$.

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