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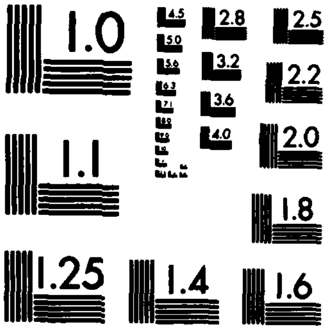

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LATTICE STATISTICS

INTERIM SCIENTIFIC REPORT

GRANT AFOSR-81-0192, 1 JUL 82-30 JUN 83

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RESEARCH OBJECTIVES AND ACCOMPLISHMENTS

The object of this research project is to develop and investigate the mathematical formalism necessary to determine occupational and neighbor degeneracies for particles distributed on lattice spaces.

The fundamental problem in lattice statistics is the determination of such quantities as the appropriate degeneracies, expectation, normalization and generating functions that arise when correlation exists among particles distributed on lattice spaces. The correlation may take many forms such as when the particles are dumbbells (occupying two adjacent lattice spaces), λ-bell particles (occupying λ linearly contiguous lattice sites) or more general factal particles that may occupy a number of contiguous lattice sites arranged in some specific form. In addition, the correlation may be in the pairing of the particles into nearest, next-nearest, etc. neighbor pairs. A further generalization of this problem concerns the situation when more than two kinds of particles are involved.

The appropriate degeneracies for any of these systems have never been obtained for lattice spaces of more than one dimension and in some cases the degeneracies are not known even for one dimensional lattice spaces.

(A) The dumbbell, λ-bell particle problem

A k^{th} neighbor pair, formed by a specific linear sequence of (k+1) particles and vacancies may be regarded, itself, as a particle that occupies more than one (say λ) linearly contiguous site on the lattice space. By considering the constrained statistics of such particles in a subspace may give us some insights into a solution of the general k^{th}-neighbor degeneracy problem.

Working along these lines has produced degeneracy algorithms describing, exactly, nearest and next nearest neighbor degeneracies for pairs of particles ($\lambda = 2$), for composite particles of any value of λ and for composite particles with identifiable ends.

Recently we have developed set theoretical arguments that permit us to obtain exact recursion relationships for the occupational degeneracy in quasi-two and three dimensional lattice spaces for λ-bell particles. The newly developed combinatorics function technique of Phares holds some hope that these multi-term, multi-variable recursions can be solved without recourse to generating functions. We expect that these techniques will facilitate the treatment of the related nearest neighbor problem in spaces of higher dimensionality. We also are attempting to compare our technique with the transfer matrix approach and other matrix approaches.

(B) The composite k^{th} neighbor problem

The other fundamental problem encountered in the mathematical treatment of lattice statistics is that of determining the composite degeneracy associated with the k^{th}-neighbor pairs created when simple, indistinguishable particles are distributed on a lattice space. [Here k designates the order of the neighbor pair, i.e., $k = 0$ corresponds to particle occupation, $k = 1$ to nearest neighbor pairs, $k = 2$ to next nearest neighbor pairs, etc.]

Stated succinctly, the problem is as follows: Given a lattice space consisting of $M \times N$ equivalent sites on which are distributed q simple, indistinguishable particles, determine the multiplicity of those arrangements characterized by a subset of the k^{th}-neighbor pairs. [Note, for example, that the "composite" degeneracy for one dimensional lattice spaces is specified by a subset of the entire set of the various kinds of k^{th}-neighbor pairs, e.g. there are six kinds of next nearest neighbor pairs ($k = 2$), 111, 110, 101, 010, 001 and 000.] In general, there are N_k, k^{th}-neighbor pairs where

$$N_k = 2^k + 2^{[k/2]}$$

in which [k/2] is the largest integer contained in k/2. Here we neglect reflective degeneracies, i.e., we count 110 but not 011.

We have developed and utilized general set theoretic arguments to generate recursion relations that yield exactly the composite nearest neighbor degeneracies for 1 x N and 2 x N lattice spaces. In addition, we have exploited these results in papers dealing with adsorption and the expectation of n_{11}, the number of occupied nearest neighbor pairs.

A related problem concerns the complete nearest neighbor degeneracy arising when more than one kind of particle [each occupies a single site] is distributed on the lattice. The importance of this approach stems from its relationship to statistical considerations arising from the mapping of one dimensional lattice spaces into subspaces in which one develops the conditional statistics of "super particles" formed from the contiguous groups of particles in the initial lattice space. In such a subspace some of the "super-particles" cannot form nearest neighbor pairs with themselves but can form nearest neighbor pairs with other kinds of "super particles." Repeated application of a mapping procedure transforms higher order neighbor pairs into "super particles" in a subspace but only at the expense of creating more, different kinds of "particles." In treating such "particles" statistically one must be cognizant of the additional constraints imposed by the mapping procedure(s).

With such mapping schemes in mind, we have been able to determine exactly, the null nearest neighbor pair degeneracy when three different kinds of indistinguishable particles are distributed on a one dimensional lattice space. This approach involves the use of operators that serve to insert particles of a specific kind into a specific sequence of particles thereby generating new, statistically allowable sequences. Such an approach leads to a matrix formulation of the problem that leads to the construction of an appropriate generating function. Specifically, we wish to generalize results obtained thus far, i.e., to determine the complete nearest neighbor pair degeneracy for an arbitrary number of indistinguishable particles on a completely filled space. Recently we have reformulated the problem along lines suggested by our previous work. It appears that this may be a fruitful approach. If we can solve the constrained statistical problem in these subspaces, an inverse mapping procedure will yield the desired degeneracy in the original lattice space.

The k^{th}-neighbor pair degeneracy problem may also be viewed as a statistical problem involving a mixture of particles having various values of λ (see above) and different internal structures. An examination of the parastatistics of such situations may yield additional insights into the complete k^{th}-neighbor degeneracy problem.

PUBLICATIONS

During the previous year [1 July 1982 to 30 June 1983] four manuscripts have been completed and one is in preparation.

1. Occupational Degeneracies for Indistinguishable Dumbbells on Saturated Two Dimensional Lattice Spaces (accepted in Discrete Mathematics).

Recursion relationships are developed that describe exactly the orientational degeneracy for indistinguishable dumbbells distributed on a $M \times N$ lattice space [for $M = 1$ through 10]. The resulting recursions yield polynomials that display a quasi-symmetry which reflects the fact that their roots exist in reciprocal pairs [or in negative reciprocal pairs]. Fundamental differences appear in the structure of these polynomials for even and odd values of M.

2. An Exact Recursion for the Composite Nearest Neighbor Degeneracy for a $2 \times N$ Lattice Space (submitted to the Journal of Mathematical Physics).

In this paper we develop set theoretic techniques that permit us to obtain a fourteen term recursion relationship that yields exactly the composite nearest neighbor degneracy for simple, indistinguishable particles distributed on a $2 \times N$ lattice space. We have also treated the associated generating functions as well as the expectation of the resulting statistics.

3. The Adsorption of Simple Particles on a $2 \times N$ Lattice Space (submitted to Surface Science).

Utilizing the recursion developed under 2.) above we have calculated the adsorption isotherm for simple particles distributed on a $2 \times N$ lattice. We show analytically that the lattice coverage exhibits no discontinuity with the gas phase pressure, i.e., no phase transition can occur in such a system.

4. The Mixed Nearest Neighbor Degeneracies on a $2 \times N$ Lattice Space (to be submitted to the Journal of Combinatorial Theory).

In this paper we determine the multiplicity of arrangements of q simple particles on a $2 \times N$ lattice that are characterized by the specification of the number of mixed nearest neighbor pairs. The associated generating functions as well as the expectation of n_{01} are also treated.

5. The Occupation Degeneracy for Dumbbells on a $3 \times 3 \times N$ Lattice Space (to be submitted to Statistical Physics).

The $3 \times 3 \times N$ lattice is the simplest space in which the coordination of some of the sites is that of a three dimensional lattice. Consequently, it is important to develop the occupation degeneracy of this space. We have developed a recursion that yields exactly the multiplicity of dumbbell arrangement. Our discussion also includes a treatment of the occupational degeneracy for dumbbells on a saturated $3 \times 3 \times N$ lattice.

TECHNICAL PERSONNEL

In addition to the principal investigator the following personnel have worked on this grant. The University of Wisconsin-Milwaukee has supported some of these people as part of this matching commitment.

1. Dr. Jeff Hock — Postdoctoral Student

   Dr. Hock has been extremely helpful in the analytic and computational parts of our research on correlated particles.

2. Ms. Deborah Swarthout — Graduate Research Assistant

   Ms. Swarthout is a physics graduate student who has worked on the research pertaining to the analytic treatment of the third nearest neighbor problems.

3. Mr. Dale Walikainen — Graduate Research Assistant

   Mr. Walikainen is a physics graduate student who is working on the nearest neighbor degeneracy problem for dumbbells with indistinguishable ends.

4. Mr. John Maeder — Undergraduate Research Assistant

   Mr. Maeder has helped with computer programming and calculations necessary for the project.

5. Mr. Tomo Radojicic — Undergraduate Research Assistant

   Mr. Radojicic is working on some computer calculations pertaining to the null nearest neighbor problem.

COUPLING

1. Dumbbell Statistics

(a) R. B. McQuistan, University of Wisconsin-Milwaukee

(b) Correspondence

(c) Discussed the use of the combinatorics function with Professor A. J. Phares, Department of Mathematics, Villanova University

2. Nearest Neighbor Statistics

(a) J. L. Hock, Marquette University

(b) Discussion

(c) Discussed some computer techniques with Professor Martin Seitz, Marquette University.

3. Recursion Polynomials

(a) R. B. McQuistan, University of Wisconsin-Milwaukee

(b) Discussion and collaboration

(c) Continuing discussions on the roots of symmetric and anti-symmetric polynomials that arise in dumbbell statistics with Professor R. L. Hall, Department of Mathematics, University of Wisconsin-Milwaukee.

4. Phase Transitions

(a) R. B. McQuistan, University of Wisconsin-Milwaukee

(b) Seminar

(c) Presented seminar on two dimensional phase transitions to Laboratory for Surface Studies.

5. Correlated Statistics

(a) R. B. McQuistan, University of Wisconsin-Milwaukee

(b) Discussion

(c) Held discussions on nearest neighbor statistics with Dr. J. M. Charain, Visiting Professor, Marsailles, France.

6. Epitaxy and Crystal Growth

(a) R. B. McQuistan, University of Wisconsin-Milwaukee

(b) Discussion

(c) Engaged in discussions on the use of lattice statistics to describe epitaxial crystal growth in two dimensions with Professor J. H. Van der Merwe, Department of Physics, University of Pretoria.

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18. SUBJECT TERMS *(Continue on reverse if necessary and identify by block number)*: Lattice statistics; nearest neighbor degeneracy; dimer statistics; correlated particles; phase transitions; cooperative phenomena; recursion relationships; (CONTINUED)

19. ABSTRACT *(Continue on reverse if necessary and identify by block number)*

The objective of this research is to develop the mathematical formalism necessary to treat correlative statistics for lattice spaces. Toward that goal the investigators are considering (1) the composite k^{th} neighbor degeneracy problem for indistinguishable particles distributed on one dimensional rectangular lattice space; (2) the occupational degeneracy for dumbbells and λ-bell particles on saturated and unsaturated, rectangular lattice spaces of higher dimensionality [here they are considering dumbbells that may have either indistinguishable or distinguishable ends]; (3) the nearest neighbor degeneracy problem for simple, indistinguishable particles distributed on rectangular lattice spaces of higher dimensionality.

A secondary objective is to exploit the results of the foregoing research by investigating the consequences of this formalism to chemical and physical systems. Most notably they are considering adsorption processes. (CONTINUED)

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22a. NAME OF RESPONSIBLE INDIVIDUAL: Dr. Robert T. Smythe

22b. TELEPHONE NUMBER *(Include Area Code)*: (202) 767- 5028

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ITEM #11, TITLE: LATTICE STATISTICS, INTERIM SCIENTIFIC REPORT, GRANT AFOSR-81-0192, 1 JUL 82-30 JUN 83.

ITEM #18, CONTINUED: Fibonacci numbers; second neighbor degeneracy; third neighbor degeneracy; occupational degeneracy; λ -bell particles; combinatorics functions; symmetric polynomials.

ITEM #19, CONTINUED: The investigators have developed set theoretic arguments that hold the promise of treating successfully a number of problems concerning correlative statistics for lattice spaces. Utilizing this technique they have been able to describe exactly the occupational degeneracy for correlated particles such as dumbbells and λ -bell particles distributed on lattice spaces of two and three dimensions.

The investigators have also utilized these set theoretic arguments to obtain recursion relations that yield exactly the composite nearest, next nearest and third nearest neighbor degeneracies for simple particles distributed on rectangular lattice spaces of higher dimensionality. Progress has also been made in utilizing the foregoing results in connection with the combinatorics function technique, to obtain explicit, analytic expressions for the appropriate degeneracies.

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