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Development Of The Applied Mathematics Originating From The Group Theory Of Physical And Mathematical Problems

James Hyman*, William Beyer, James Louck, and Nicholas Metropolis

Abstract

This is the final report of a three-year, Laboratory-Directed Research and Development (LDRD) project at the Los Alamos National Laboratory (LANL). Group theoretical methods are a powerful tool both in their applications to mathematics and to physics. The broad goal of this project was to use such methods to develop the implications of group (symmetry) structures underlying models of physical sytems, as well as to broaden the understanding of simple models of chaotic systems. The main thrust was to develop further the complex mathematics that enters into many-particle quantum systems with special emphasis on the new directions in applied mathematics that have emerged and continue to surface in these studies. In this area, significant advances in understanding the role of SU(2) 3nj-coefficients in SU(3) theory have been made and in using combinatoric techniques in the study of generalized Schur functions, discovered during this project. In the context of chaos, the study of maps of the interval and the associated theory of words has led to significant discoveries in Galois group theory, to the classification of fixed points, and to the solution of a problem in the classification of DNA sequences.

1. Background and Research Objectives

This final progress report is presented in three parts to show its distinct components, but it is emphasized that the common theme linking these subjects is group theoretical methods, a discipline in which all the co-investigators have experience. All subjects discussed here have a long history of support in the Laboratory with numerous contributions from the co-investigators.

a. Spectroscopy and Symmetry. The term spectroscopy encompasses the broad class of problems in all of quantum physics whose goal is to calculate energy levels of complex many-body systems and transition amplitudes for such systems in interaction with radiation

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and other fields. This includes particle, nuclear, atomic, and molecular physics and chemistry. A principal tool in spectroscopy is the implementation of symmetry. In a broad sense, symmetry incorporates and systematizes the intrinsic geometry of large classes of physical systems. This common information can be calculated and stored once and for all as theoretical progress is made . This allows otherwise unwieldy calculations to focus on the particular physics that distinguishes a given system of interest.

The mathematical tool for implementing symmetry is group theory, which includes group representations (because quantal systems are described in Hilbert space) and a wide class of coefficients [generalized Wigner-Clebsch-Gordan (WCG) and Racah coefficients] for reducing Kronecker products of groups and constructing invariants. Kronecker products of groups are the mathematical technique for implementing the fundamental notion that complex systems are built-up from simpler ones. Accordingly, spectroscopy, in this broad sense, is an integral part of any research laboratory having programs based on modern quantum theory.

b. Combinatorics and Invariant Theory. The study of hypergeometric series is a classical branch of mathematics originating with Gauss and developed further during the last and early part of this century. Combinatorics and invariant theory are also rooted in this same time frame, but have undergone a revitalization and rigorous treatment during the last twenty years in the hands of Rota (MIT) and others. A merging of these two fields has recently been brought about by discoveries of Biedenharn and Louck **[1-3]**, and still more recently with the help of Chen **[4]**, through the concept of generalized Schur functions and generalized hypergeometric series rooted in the physical theory described in (a) above.

c. Iteration Theory. The classification of all cycles of the parabolic map (not just the stable ones under forward iterations) is an important problem in iteration theory. A preliminary paper was published on this by Bivins, Louck, Metropolis, and Stein **[5]**, and a second paper giving the complete solution of this difficult problem, using a combination of computer and theoretical insights, is now near completion **[6]**. The early studies of the parabolic map, and the discovery of universal maps, began at this Laboratory with a seminal paper by Metropolis, Stein, and Stein in 1973. This work has continued over the years through the activities of a small, dedicated group of investigators, including most of the names mentioned in this report. The foundation of the Laboratory's Center for Nonlinear Studies was influenced by this early work on chaos. The continued work on fundamental aspects of this problem by Beyer, Bivins, Louck, Metropolis, and Stein brings a great deal of compatible experience and power to this problem. Beyer and Louck **[7]** completed a fundamental paper in 1994 on infinite families of solvable Galois groups, a subject that probably could not have been addressed without the legacy of its roots in Los Alamos. A similar assessment may be made of the classification of fixed points into cycles by Bivens, et al.

2. Importance to LANL's Science and Technology Base and National R&D Needs

This work has contributed to the general base of knowledge important for the general intellectual vitality of the nation and, in particular, of this Laboratory. Students and university lecturers come to this Laboratory because they know they can interact effectively and challengingly with its staff. Some stay. Potentially, in the longer-term, some of this work can influence methodologies in the several fields to which it relates. More significantly, if an applied mathematics effort at the Laboratory is to be successful, it must have the respect of all its peers. The work reported here has contributed substantially to that.

3. Scientific Approach and Results

Let us review the principal areas of research and the significant results and papers that have come out of this proposal during its three years of existence.

a. Cycles of Iterate of Parabolic Maps. Major progress was made in classifying all cycles of the nth iterate of the parabolic map **[5, 6]**. This problem entails a complete description of a set of inverse functions of the nth iterate. These functions are labeled by words on two letters. A certain distinguished subset of all such words provides labels to what are known as cycle classes. These cycle classes partition the set of all words into equivalence classes. We proved earlier the existence and found the actual assignment of these distinguished words, which, in turn, are used toward giving the complete description of all the bifurcation properties of the parabolic map **[5, 6, 8]**.

The set of fixed points of the nth iterate of the parabolic map on the interval may be decomposed into sets of cycles of the parabola. This decomposition is of unsuspected difficulty and richness in structure. It contains, for example, all the stable limit cycles for forward iteration, and, in addition, all stable limit cycles for inverse iterations. We (Bivins, Louck, Metropolis, Stein) have learned the general rules for effecting the general decomposition, this leading to significant new applications of the famous Möbius inversion formula. The most significant result has been the proof of a theorem that describes, beautifully for all n, the intervals in parameter space in which a bifurcation occurs, either of the tangent or period-doubling type. This theorem gives the solution of the problem and accomplishes one of the major goals of this work. Also, an advancement in the Feigenbaum theory of period doubling has been made. Li Wang, with help from Beyer, has finished a proof of the quadratic convergence in period doubling for the trapezoid map **[9]**. This phenomenon is quite different from the linear convergence obtained for Feigenbaum's parabolic map. This is an important result because it shows that convergence properties are not universal.

A final paper setting forth a comphehensive theory is in preparation **[6]**.

b. Galois Theory Applied To Iterates of the Logistic Map. The second major accomplishment was in completing the description of the Galois group of an important equation associated with the nth iterate of the parabolic map. This problem is particularly intriguing because the polynomials depend on a parameter so that in effect one is studying infinite sets of polynomials and Galois groups. The proof that the Galois group for general parameter is the n-fold wreath product group of the symmetric group on two objects, and the realization of that group as permutations, was a significant result. That for the special parameter value 2 the Galois group collapses to the cyclic group was also proven using properties of the Chebyshev polynomials and some associated number theoretic results. A preliminary paper on these results was presented by Beyer at the Ulam Conference in Florida and the completed work was published in the Ulam Quarterly in 1994 [7]. A further report on the work was given at the European Conference on Iteration Theory held at Opava, Czech Republic in August 1994.

c. Arbitrary Power of the Companion Matrix. Chebyshev polynomials have important applications to approximation theory and to finite field theory. Stimulated by the occurrence of the polynomials in iteration theory (item b above), Louck and Chen **[10]** considered their generalization to n variables. This resulted in a remarkable formula giving explicitly all elements of the n-th power of an m x m matrix known as the companion matrix. The resulting polynomials were later learned to be known as Dickson polynomials, since they were studied in the dissertation of Dickson at the turn of the century. To our surprise, we learned that a whole book has been devoted to Dickson polynomials by R. Lidl, G. L. Mullen, and G. Turwald (John Wiley, 1993), but the beautiful synthesis of properties given by the Chen-Louck formulation was not known. The paper was accepted almost immediately for publication, and P. J.-S. Shiue, an expert in this field, said it was the most important contribution to his field that he had read.

d. 3n-j Coefficients and SU(3) Symmetry. A major discovery was made for the theory of the WCG coefficients of the unitary group SU(3), one of the important symmetry groups having applications across all areas of physics (particle, nuclear, atomic, chemistry). This was that the multiplicity of irreducible representations in the Kronecker product may be enumerated by a triangle of angular momentum labels associated with the group SU(2). This stimulated a review of previous work with the resulting consequence that the so-called 9-j invariant operators and the associated 9-j coefficients are at the root of the structure of the U(3):U(2) invariant operator structure of the WCG coefficients of SU(3). This is a significant result for understanding these complex objects. This work was reported on by Louck in three lectures given at a conference in Zajacykowa , Poland during the week of September 1-7, 1994 and appears in the proceedings of the conference **[11]**.

e. Reference Book Work. Louck [12] has completed a lengthy (over 50 pages) review of the angular momentum theory to be included in a major Reference Book to be published in 1995 by the Atomic, Molecular, and Optical Division of the American Physical Society.

f. Stochastic Algebra Applied to a Problem in Genetics. An application of genetic algebra has been made to the problem of calculating probabilities in each generation of the number of gene types in a Mendelian mating scheme with three gene types: dominant, mixed, and recessive. An explicit formula is given for these probabilities as a function of the generation number. The derivation used a nontrivial induction procedure **[13]**.

g. Related Work. Unfinished work continues with Pedersen in a paper on "Vectors of zero length and solutions of Laplace's equation in Rn" and related methods for solving differential equations **[14]**.

h. Relation of Unitary Symmetry Functions to Combinatorics. One of the major goals of this project was to give the various functions that appear in the study of unitary symmetry (irreducible representation functions, discrete functions related to the reduction of Kronecker products, and unitary invariant functions, both continuous and discrete) a firm basis in combinatorics. A good start has been made in that direction through collaborations with William Y.C. Chen, not only in the earlier work on generalized Schur functions **[4]** and the companion matrix **[10]**, but more recently in three additional papers: one relating unitary representations of groups to the famous MacMahon Master Theorem of combinatorics and to Rota polynomials arising in the double-tableau calculus **[15]**; a second giving a generalization of the Lagrange interpolation formula to symmetric functions **[16]**; and a third revealing the structure of generating functions for 3n-j coefficients as functions defined on the vertices and lines of their associated cubic graphs **[11]**. These three papers set the stage for continued work in this area under the more general mathematical framework of combinatorics.

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