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COMPUTATIONAL AND GROUP-THEORETICAL METHODS APPLIED TO THE SOLUTION OF QUANTUM MECHANICAL WAVE EQUATIONS

By

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TO

Evodio Carlos

I. INTRODUCTION

It is a prevalent and generally accepted notion that the physical and chemical properties of matter can be deduced by solving Schrödinger's equation or one of its relativistic or field-theoretic generalizations such as the Dirac equation or the Bethe-Salpeter equation. To the extent that such ideas are correct, it would seem that our understanding of the fundamental aspects of physical phenomona must depend upon our ability to handle such equations. This is no easy matter, even for very simple and highly idealized models, with the result that progress in the material understanding of Nature requires a continual refinement of mathematical techniques. Particularly with the advent of electronic computation in the past two decades it has become possible to analyze models of a complexity previously inaccessible, on a scale largely determined by the speed, accuracy, and information storage capacity of the available computer. Although these parameters ultimately set limits upon the scope of any investigation, the value to be gained from exploiting resources such as electronic computers depends considerably upon an understanding of their capabilities and characteristics, quite beyond any understanding necessary for the problem being solved itself.

Some aspects of understanding and simplifying the quantum mechanical wave equations, together with some experiences in attempting to employ computers in an organized and disciplined fashion to advance this understanding still further, are the themes of this dissertation, which is based upon the series of published articles which are listed in Section II. They are designated in the text by references of the form D-k, and seem to fall into three groups, which it is convenient to discuss individually.

Matrix Hamiltonians, Finite Groups, and Matrix Algebra
Computation
Quantum Mechanical Wave Equations

By a matrix Hamiltonian we mean a Hermitean, usually real, matrix which we intend to diagonalize. Its origin will generally be as the Hamiltonian in some finite model such as the Hückel theory, or as a matrix which plays an equivalent role, such as those arising in small vibration theory.

The first group of papers is representative of techniques which are mostly algebraic in character; those of the third part depend mainly upon the properties of differential equations and their analytic character. To the extent that they involve algebra, it is through Lie groups and Lie algebras. In the first and third categories one can recognize the concrete character of the scholarly literature, as it has acquired a definite form for well more than a single century. In dealing with electronic computers one enters a field qualitatively different from the traditional areas of study, publication, and discussion. In scarcely two decades these machines can hardly be supposed to have reached the beginnings, much less the limits, of their technical development. Nevertheless it is possible to see some trends emerging which will establish a class of machines which may well stabilize into a prolonged existence, even if further engineering and technological advances someday lead to memory stores or processing speeds orders of magnitude beyond what is presently available.

As a practical matter, however, computation involves some politico-economic problems which are more severe than those in more sedate areas of research. Nor can one always state his conclusions in the neat form of theorems. Nevertheless in the second part of the dissertation there are described four progressively more successful schemes for organizing, as distinguished from performing, one's programming tasks.

Although the dissertation summarizes the contents of the papers listed in section II, establishes their relation to one another, and outlines the general context in which they were written, considerations of space preclude either an elaborate historical account or critical analysis of the fields in which they lie. Many of the articles contain their own historical introduction, although related articles have inevitably come to light after the date of publication, and there have been noteworthy advances since some of the older articles were written. It might be noted that the article D-21 is itself such a survey and analysis of symmetry and degeneracy in Hamiltonian mechanics, covering the period up to the end of 1968, and that it includes within its purview the remaining articles of the third group.

II. LIST OF PUBLICATIONS

D-1 Harold V. McIntosh, "Towards a Theory of the Crystallographic Point Groups", Journal of Molecular Spectroscopy *5*, 269–283 (1960).

D-2 Harold V. McIntosh, "Symmetry Adapted Functions Belonging to the Symmetric Groups", Journal of Mathematical Physics *1*, 455–450 (1960).

D-3 Harold V. McIntosh, "On Matrices which Anticommute with a Hamiltonian", Journal of Molecular Spectroscopy *8*, 169–192 (1962).

D-4 Harold V. McIntosh, "Symmetry Adapted Functions Belonging to the Crystallographic Groups", Journal of Molecular Spectroscopy *10*, 51–74 (1963).

D-5 Harold V. McIntosh, "Virtual Symmetry", Journal of Molecular Spectroscopy *13*, 132–147 (1964).

D-6 Enrique Daltabuit and Harold V. McIntosh, "Representations of the Magnetic Symmetry Groups", Revista Mexicana de Fisica *16*, 105–114 (1967).

D-7 Adarsh Deepak, Victor Dulock, Billy S. Thomas and Harold V. McIntosh, "Symmetry Adapted Functions Belonging to the Dirac Groups", International Journal of Quantum Chemistry *3*, 445–483 (1969).

D-8 Jesús Ortega Campos, Isidro Romero Medina, Evodio Lopez Rojas, Leonel Torres Hernandez and Harold V. McIntosh, "Lattice Dynamics with Second Neighbor Interactions", International Journal of Quantum Chemistry Symposium *5*, 201–225 (1971).

D-9 Harold V. McIntosh, "An Experiment on Teaching the Use of Large Electronic Computers", The American Mathematical Monthly *70*, 207–209 (1963).

D-10 Adolfo Guzman and Harold V. McIntosh, "CONVERT", Communications of the Association for Computing Machinery *9*, 604–613 (1966).

D-11 Adolfo Guzman and Harold V. McIntosh, "Comments on 'All Paths through a Maze' ", Proceedings of the IEEE *55*, 1525–1527 (1967).

D-12 Harold V. McIntosh, "A CONVERT Compiler of REC for the PDP-8", Acta Mexicana de Ciencia y Tecnologia *2*, 33–43 (1968).

D-13 Harold V. McIntosh, "On Accidental Degeneracy in Classical and Quantum Mechanics", American Journal of Physics *27*, 620–625 (1959).

D-14 V. A. Dulock and Harold V. McIntosh, "On the Degeneracy of the Two-Dimensional Harmonic Oscillator", American Journal of Physics *33*, 109–118 (1965).

D-15 V. A. Dulock and Harold V. McIntosh, "Degeneracy of Cyclotron Motion", Journal of Mathematical Physics *7*, 1401–1412 (1966).

D-16 V. A. Dulock and Harold V. McIntosh, "On the Degeneracy of the Kepler Problem", Pacific Journal of Mathematics *19,* 39–55 (1966).

D-17 Arturo Cisneros and Harold V. McIntosh, "Symmetry of the Two-Dimensional Hydrogen Atom", Journal of Mathematical Physics *10*, 277–286 (1969).

D-18 Manuel Berrondo and Harold V. McIntosh, "Degeneracy of the Dirac Equation with Electric and Magnetic Coulomb Potentials", Journal of Mathematical Physics *11*, 125–141 (1970).

D-19 Arturo Cisneros and Harold V. McIntosh, "Search for a Universal Symmetry Group in Two Dimensions", Journal of Mathematical Physics *11*, 870–895 (1970).

D-20 Harold V. McIntosh and Arturo Cisneros, "Degeneracy in the Presence of a Magnetic Monopole", Journal of Mathematical Physics *11*, 896–916 (1970).

D-21 Harold V. McIntosh, "Symmetry and Degeneracy", *in* GROUP THEORY AND ITS APPLICATIONS, Volume 2 (Ernest M. Loebl, Editor), Academic Press, New York, 1971, pp. 75–144.

III. MATRIX HAMILTONIANS, FINITE GROUPS, AND MATRIX ALGEBRA

The first group of publications is probably best characterized by its algebraic nature, symbolic intent, and its applicability to finite matrices and finite groups. Insofar as possible the algebraic eigenvalue problem is organized and simplified by exploiting auxiliary properties of the Hamiltonian. Experience has shown that the following topics and techniques might well be considered.

decomposition of the matrix as a tensor product
symmetry, especially hidden symmetry
projection operators and irreducible representations
special commutation relations within sets of matrices
special relations between the eigenvalues of a matrix
virtual symmetry and the possibility of embedment
partitioning into submatrices
the special properties of band matrices
the dependence of eigenvalues and eigenvectors on parameters
eigenvalue bounds, interleaving and clamping theorems
residual degeneracy
location of critical points in the spectral function
perturbation theories
the properties of positive or definite matrices.

Not all of them are touched upon in the publications of this dissertation, and some represent areas of voluminous publication by other authors; however when taken in the order presented they serve as a kind of checklist whereby it is possible to encounter some simplification if it exists. Otherwise it would be necessary to resort to a numerical calculation, or a lengthy analytic investigation. Even then, if some degeneracies went undetected, the convergence of a numerical process would surely suffer.

A. Decomposition of a matrix as a tensor product

Occasionally a matrix may be decomposed as a direct sum, tensor product, composite matrix, or other specialized form. Such possibilities should always be kept in mind, although in practice they are usually either thoroughly obvious from the outset or else the end product of another process. Tensor products are usually associated with multidimensional problems and arise where one might expect a separation of variables. Direct sums are the usual goal of symmetry factorizations. Imprimitive matrices are especially important for their connection with induced representations.

B. Symmetries, Especially hidden symmetries

The use of group representation theory in simplifying secular equations is very old and certainly very widely used (1). Its importance depends upon the fact that matrices commute if and only if they define a mutually compatible splitting of their vector space into stable subspaces. It is possible to consider larger sets of matrices than a single pair. According to Burnside's theorem, only a multiple of the unit matrix can commute with an irreducible set, while Schur's lemmas determine the commuting algebra in the case where the matrices form a reducible representation of a Group.

To benefit the most from having a symmetry group one ought to have the largest group possible, but sometimes a lesser one will be chosen. Whatever the group, Schur's lemmas lead to a tensorial product form for the group's representation, requiring any commuting matrix to have the complementary tensorial form. From this requirement follows an enforced eigenvalue degeneracy and the noninteraction of eigenvectors of different symmetry types, which is the relation between symmetry and degeneracy for which group theory is so renowned. The possibility of "accidental degeneracy" or "hidden symmetry" arises from having missed fully anticipating one or the other of these two aspects of the physical situation described by the matrix.

Hamiltonian mechanics is prone to the occurrence of hidden symmetry because of the tendency to regard problems which must be formulated in phase space only in terms of configuration space, so that the symmetry between coordinates and momenta inherent in many systems, foremost of all the harmonic oscillator, is overlooked. Such omissions are much rarer in problems of molecular or lattice dynamics, or finite approximations to the Schrödinger equation such as one finds in the Hückel theory, but can

sometimes occur when one pays inadequate attention to the freedom of movement possible in these systems. The symmetry of "non-rigid" molecules may be an example, especially when nearest neighbor interactions only are taken into account (2).

In another direction, the elimination of the translational or rotational variables for the whole molecule, as is habitually done in molecular spectroscopy, is never based on the Euclidean symmetry which is clearly responsible, although it is not so clear whether there would be much point in classifying the remaining degrees of freedom according to their Euclidean symmetry type.

C. Projection operators and irreducible representations

Having selected a symmetry group, albeit the obvious and traditionally accepted one, it must still be put to use, generally by constructing its projection operators. But alternatively, the character table, group multiplication table, class lists, or some other data may be desired. There are two obstacles to obtaining them. It is redundant to say that larger groups have more elements; the difficulty is that groups grow by acquiring more generators, multiplying rather than adding to the order of the group. The second obstacle is that Hamiltonian matrices, for example those encountered in spin-wave theory, may possibly be of enormous dimensionality even though their symmetry groups remain relatively small.

There will always be a premium for reducing the number of matrices to be dealt with, and for simplifying their form. Imagine the saving, could it be shown that the representation matrices were tensor products, if only the tensorial factors were required, and at that, only those which were associated with the generators of the group.

M. A. Melvin (3) observed empirically that the projection operators for a very many groups could be factored. The intent of D-1 was to show that this factorization was a consequence of the semidirect product nature of the groups involved. At the same time Löwdin (4) had obtained a very curious result wherein he obtained projectors for angular momentum states by methods which strongly suggested the projection operators of the symmetric groups. This equivalence was demonstrated in D-2, which also established a

rather special factorization involving Young's symmetrizers α and β. When applied to an element x, one should expect the projection to be accomplished by the product $\alpha\beta \times \alpha\beta$, whereas only $\alpha \times \beta$ is required, allowing the projection operator to be "split".

The program set forth in D-1 was realized for all symmomorphic groups in D-4. The difficulty for the non-symmomorphic groups lies in the fact that their representations are obtained by a recursive process which requires projective representations of a factor group at one point. Unfortunately, this projective representation may turn out to be just the ordinary representation of the larger group which we are seeking, rendering the process useless.

Perhaps the most significant aspect of the results contained in D-1 and D-4 is the factorization of the row projection operator in the fashion envisioned by Melvin, and earlier by Fokker (5). As a method it seems to be basically sound; one might compare the fantastic success that has been enjoyed by the *fast fourier transform* (6), a quite similar process invented for abelian groups.

During the years which have transpired since the writing of these three articles, it has become clear that the essence of their projection operator factorizations is not that they apply to direct or semidirect product groups, but that they apply to *induced representations.* Because representations induced from normal subgroups are generally far simpler to handle the results were much more evident for semidirect product groups.

D. Sets of matrices satisfying special commutation relations

The use of symmetry groups is no doubt the most widely used aid in the simplification of matrix Hamiltonians. Yet, it is not so necessary to have a full group, although the presence of one is conducive to much more elegant theorems. Whatever the collection of operators, it is their irreducibility which matters, and this in turn can be dealt with through Burnside's theorem.

Continuing in the same line, it can be said that any theoretical justification for splitting a space into Hamiltonian-stable subspaces would be quite helpful, but not really necessary. It would even suffice to isolate a family of subspaces over which the Hamiltonian acts transitively. One way to achieve this would be for the Hamiltonian to be a member of a set of matrices which satisfy some algebraic relationships. For finite matrices this

is the equivalent of having a dynamical group for general Hamiltonians.

A very simple and quite usable algebraic relation is a commutation rule,

$$H A = \omega A H,$$

of which anticommutation is the special case for $\omega = -1$.

Consequences of this relationship are examined in detail in D-3, an article which was motivated by a desire to explain Coulson's (7) discovery of negative eigenvalue pairing in certain Hückel Hamiltonians pertaining to alternant hydrocarbons. It was generalized for complex multipliers after the discovery that Rudenberg (8) had anticipated the result for -1 as a multiplier. A further generalization was taken in D-7 by considering an entire family of operators ω_{ij} wherein

$$H_i H_j = \omega_{ij} H_j H_i .$$

Such a family generalizes the matrices familiar from Dirac's relativistic theory of the electron, and also establishes all the projective representations of finite abelian groups. From another viewpoint, we could say that a commutation relation such as this defines a projective symmetry, in which a multiple of the Hamiltonian is recovered from a change of coordinates. The projective symmetries are induced by the normal subgroup of traditional symmetries.

Projective representations of abelian groups are of interest as magnetic space groups. Some slight generalizations were explored in D-6.

E. Matrices with special relations between their eigenvalues

The algebraic identities which matrices satisfy determine configurations of their eigenvalues. Conversely, the configuration implies auxiliary matrices such that the appropriate algebraic identity may be realized. Thus, when the eigenvalues of H occur in negative pairs, there exists a matrix J conjugating H into its negative,

$$J^{-1} H J = -H.$$

We could equally well imagine that when the eigenvalues occur in reciprocal pairs, H could be mapped into its reciprocal,

$$J^{-1} H J = H^{-1},$$

and so on. Even non-algebraic relations, such as the mapping of an arbitrary, not necessarily hermitean, matrix into its complex conjugate or into its transpose, can occasionally be useful. Some of these combinations are fairly important for the theory of waves.

Beyond this interplay between matrix identities, the eigenvalues and the eigenvectors, there are occasions to employ the relationships more explicitly. For example, in D-3 it was shown how to write the projection operators for H in terms of those for H^2 and the anticommuting J; this is also the origin of a projection operator factorization due to Günthard (9), supposing the exchange factor to be an arbitrary k*th* root of 1. In D-8 and (10) a similar reduction was applied to a matrix whose roots occurred in reciprocal pairs.

The occurence of reciprocal pairs is characteristic of symplectic matrices, just as the occurence of negative pairs typifies the matrices of their Lie algebras. Indeed the exploitation of commutation relations and their requirements on the eigenvalues and eigenvectors of matrices reaches the height of intricacy in the classification of all semisimple Lie Algebras, but it is to be remembered that commutator bracket relationships are so regular that they define an entire self-contained algebraic system.

In looking about for mappings and eigenvalue families there is a restriction in that finite dimensional spaces can only admit a finite number of eigenvalue categories, so that the operators mapping between them must be either nilpotent or cyclic. Negatives, conjugates, reciprocals, transposes, and complex multipliers of absolute value 1 rather much exhaust the possibilities for cyclic mappings, although in the theory of angular momentum it is possible to find nilpotent mappings; viz. the ladder operators.

F. Virtual symmetry and embedment techniques

When there are special relations between the eigenvalues of a matrix, or even when it satisfies some relatively simple functional relation, it may be that

the most concise description of the matrix is to say that it behaves in a certain way when there is a change of coordinate system. Thus there is symmetry when a matrix remains unchanged by a change of coordinates. This is one way in which changes in the environment of a physical system are reflected by the mathematical properties of its Hamiltonian. Analogously we can suppose that the relationship of a system to its components will influence the relation between a Hamiltonian matrix and its submatrices. The concept of virtual symmetry depends upon the possibility that several systems may be embedded into a larger one in such a way that there is no difference in their behaviour, whether they are treated separately or collectively.

The article D-5 relates a striking example of how it may be understood that the vibrations of finite chains, as well as of rectangular and triangular membranes and such like, show such impressive resemblance to cyclic or infinite systems, which go considerably beyound the approximations involved in the use of the Born-von Karman boundary conditions.

A practical limitation for the embedment technique is that it requires the use of an isolating boundary for the subsystems, which it may not always be possible to construct. Thus, it is not the way to analyze such things as the vibrations of irregular membranes, or chains with far neighbor interactions. Nevertheless there are accidental degeneracies occurring in the vibrations of far-neighbor chains which can be explained by noting that their normal modes can be imbedded in the vibration of a cyclic chain, whereas the nondegenerate modes cannot. In this case the embedment is a condition for degeneracy and the hidden symmetry is a virtual symmetry.

G. Partitioning techniques (11)

More often than not a system will lack an isolating boundary which will create a virtual symmetry, but it is nevertheless convenient to be able to interrelate the properties of a system and those of one or more subsystems. The partitioning technique, as elucidated by Löwdin and subsequently exploited in many contexts, provides an especially systematic method whereby this is possible. It is particularly useful when a one-dimensional subspace is to be isolated, as it allows the characteristic equation to be

represented as a rational fraction in a way which is frequently very illuminating. It may also be used as a basis for the construction of effective Hamiltonians, perturbation series, and other aproximate methods.

H. The properties of band matrices

When methods destined to separate a matrix into parts such as a direct sum or a tensor product fail, and partitioning or embedment does not seem appropriate, there still remain some special forms amenable to a relatively definite analysis. For example, the band diagonal form which arises from a system which can be linearly ordered and for which the interactions between parts are limited in range. The most widely known band diagonal form is the tridiagonal form, in which interactions occur only between immediately consecutive coordinates. Since it is the first step in most numerical methods for diagonalizing symmetric matrices, it is now generally known that any symmetric matrix may be reduced to tridiagonal form. When this transformation is made, it is easy to lose sight of much information resident in the original matrix, so that theoretically it is preferable to discuss the higher band matrices in their original form.

Sturm-Liouville theorems apply to strictly tridiagonal matrices, to the effect that

1) no eigenvector can have two consecutive nodes
2) the terminal components cannot be zero
3) no eigenvalue can be degenerate
4) the eigenvector of lowest eigenvalue has no nodes
5) the eigenvalues are ordered according to the number of nodes of their eigenvectors

In D-8 it was reported that a 2n + 1-diagonal matrix generalizes these theorems in the respect that

1) no eigenvector can have 2n consecutive nodes
2) not all of the n initial or final coordinates can be zero
3) the maximum degeneracy possible is n-fold
4) the eigenvalues are not generally ordered according to their number of nodes
5) if the matrix is *positive* the lowest eigenvector may still be nodeless.

These results can be established by writing the eigenvalue equations as a recursion relation between the consecutive components of the eigenvector and then examining the eigenvalues and eigenvectors of the recursion relation. Under fairly general conditions of reflective symmetry these eigenvalues will occur in reciprocal pairs.

By using band diagonal matrices in linearly ordered systems one can avoid the approximations inherent in the Born-von Karman boundary conditions, which are the more severe, the shorter the chain. It is also curious that the highest degeneracies occur in situations of virtual symmetry, where the finite chain is embedded in a ring, which provides the hidden symmetry needed to account for the degeneracy.

I. Matrices which depend upon parameters

There may come a time when elaborate searches for symmetry principles and decomposition schemes for matrices will be accorded the same respect which now attends the desire to write formulas for the roots of algebraic equations. The quadratic formula is part of every citizen's education; it is known that such matters were once exhaustively investigated with results which only a few specialists now understand; and it is generally expected that numerical procedures will be used, in many cases even to resolve quadratic equations.

A certain parallel can surely be discerned in the application of group theory in the physical and chemical sciences. For more than three decades after the introduction of the quantum mechanical wave equations every effort was made to reduce them to ordinary differential equations in a single variable and to transform them into coincidence with one of those arising from a small number of key potentials which had not only been studied in minute detail, but which had certain very special features. As an illustration one might follow the literature of double-minimum potentials to see how research was influenced by the desire to find a tractable standard model.

Similar tendencies have overshadowed the studies of molecular spectra or solid state physics where the only hope of reducing the number of parameters and of obtaining matrices amenable to hand calculation lay in the restrictions imposed on systems of exceptionally high symmetry. Thus,

there has been a certain practical as well as aesthetic motivation in extending the exploitation of group theory and algebraic techniques as far as possible, which may diminish greatly when computers exist which handle all matrices equally.

Surely there are some aesthetic limits, for it will probably be conceded that symmetry groups whose *only* definition lies in the fact that they consist of "all the invertible matrices which commute with the Hamiltonian" are not of much utility. Indeed it is just the independent availability of symmetries that makes them useful. Here we ought to mention a process introduced by Caspers (12) which can assure degeneracy in a matrix in such a way that the symmetry group is not likely to ever have an independent description, nor is there likely to ever be more than a sporadic isolated degeneracy.

Suppose that two n-dimensional Hermitean matrices A and B are combined with the aid of a parameter k to produce a Hamiltonian matrix H,

$$H = A + k\,B.$$

Degeneracy in H can be detected by forming the Vandermonde determinant of its eigenvalues,

$$V = \prod_{i<j} (\lambda_i - \lambda_j).$$

Degeneracy occurs if and only if $V = 0$, but it is not helpful to have a criterion expressed only in terms of the eigenvalues of H. Rather one can write V^2 in terms of traces of powers of H

$$V^2 = \begin{vmatrix} \mathrm{tr}\mathbf{I}\cdot\mathbf{I} & \mathrm{tr}\mathbf{I}\cdot\mathbf{H}\ldots \\ \mathrm{tr}\mathbf{H}\cdot\mathbf{I} & \mathrm{tr}\mathbf{H}\cdot\mathbf{H}\ldots \\ \ldots & \end{vmatrix},$$

a formulation which makes it evident that V^2 is a polynomial of maximum degree $n(n-1)$ in k, whose roots always occur doubly. Thus, counting multiplicities, there are no more than $\frac{1}{2}\,n(n-1)$ values of k for which $V = 0$, unless it should happen that V would be equal to zero independently of the value of k. Not all, nor even any, of these roots need to be real, although in the case that A and B commute, they will all be real.

Applied to the example of pentadiagonal matrices, the ratio of whose diagonal bands is k, we see that there is a quota of $\frac{1}{2}$ n(n−1) degeneracies, for all possible values of k, which can be realized two at a time.

J. Eigenvalue bounds, interleaving and clamping theorems

There are many published theorems, some much more useful than others, relating to the distribution of eigenvalues, bounds upon their magnitude, and consequences upon the eigenvalues of relationships between matrices. Of principal interest in numerical investigations, such theorems can also be quite useful for theoretical purposes.

K. Residual degeneracy

One interesting way that the variation of parameters may be employed is to vary the strength of interaction between initially isolated, identical subsystems. If the isolated components are themselves highly degenerate, say on account of being especially symmetrical, the interleaving theorems will ensure that only one level is lost from each degenerate cluster for each new row of interactions which appears in the Hamiltonian matrix when they may interact. If the number of additional couplings is less than the degree of uncoupled degeneracy, some must remain, without the corresponding symmetry group having much geometric importance.

L. Critical points of a spectral function (13)

When a matrix is decomposable as a sum of tensor products, which can typically occur in multidimensional systems, there may result a formula expressing the total eigenfunction as a function of the eigenvalues of the tensorial factors. Degeneracies, generally associated with the critical points

of this spectral function, may arise from the way in which the same final eigenvalue can arise from several distinct combinations of the partial eigenvalues. An example of how a very high degeneracy can arise in this way, eventually leading to discontinuities in the distribution of frequencies for a limiting continuous system, is discussed in D-5.

M. Perturbation theories

The published literature also abounds with perturbation theories, including some interesting ones based on the partitioning technique. I have avoided discussing all approximate procedures in order to show the extent to which exact results can be obtained, but one should nevertheless remain aware of approximate and iterative techniques, especially since many of them yield excellent numerical procedures.

N. Positive matrices (14)

There are many specialized categories of matrices whose special properties can often be exploited to advantage. Matrix Theory and Linear Algebra, as it is usually taught and known to people who wish to apply such things, is based on the L^2 Hilbert-space metric. Applications, especially in probability theory, sometimes indicate a preference for the absolute value norm. These matters seem to find their most systematic development in the theory of positive matrices. Useful results include the fact that a strictly positive matrix has a unique maximum eigenvalue with a nodeless eigenvector, as well as some eigenvalue estimates and bounds. Also, an indecomposable not strictly positive matrix obeys an exchange relation, so that its eigenvalues occur in complex cycles with a uniform multiplicity.

IV. COMPUTATION BY ELECTRONIC COMPUTER

A seemingly adequate scheme for publication in mathematics or physics now seems to be well established, as it has been in most other disciplines. The field of computation is new, no more than two decades old, and by its nature has neither been conducive to scholarship nor to the traditional scheme of publication. Mathematical theorems published in the last century are still important, but one wonders how many ten-year-old computer programs are still of much value. This is not so much because the mathematical techniques which they employ have become outmoded, although there has been a continuing evolution of computer methods, nor that the problems which they were created to solve are no longer of interest. In good part it is due to the fact that the technology of computer design and construction has been envolving, and in good measure it is due to the fact that these programs were poorly planned and inadequately prepared from their outset.

It is true that the existence of large, fast, reliable electronic computers has stimulated numerical analysis, that new techniques have evolved which are much better adapted to computers than were the methods perfected for hand work, and that the computer methods themselves are acquiring an increasing sophistication. It is also true that the computing capacity which is available to any given scientific investigator in 1972 permits a depth of analysis, a breadth and scope of aproach, that the routine research of today would have been beyound any possibility whatsoever of realization in the previous generation. How strange it is today to go back and read some of the early articles (15) extolling the virtues of mechanical computation for such a rudimentary operation as cummulating sums of products, especially when one notes that the numbers are all to be punched on rectangular cards by a special machine, one per card,. . . Be it noted that an article was published on such a procedure by one of the leading chemical laboratories, of such a stature that it commanded the resources to procure such costly equipment to aid in its most pressing investigations. The suggested aplication was x-ray structure analysis. We don't know if the mentioned article resulted in any sales of the equipment which it described or any requests to use the facilities, but it truly described the equipment and the state of the art at the time of its publication.

In order to facilitate the sales of their wares, computer manufacturers have found it convenient to insist that writing a program is no more complicated than writing algebraic formulas themselves, while their clients have had a variety of reasons for accepting such declarations. Foremost of the many political, social, and economic forces which have been at work shaping the present computer scene is the need for universality. A program needs to be usable, insofar as possible, on whatsoever computer, irrespective of its brand of manufacture, to insure against the necessity to repeat laborious and costly effort in recreating programs in the event of the acquisition of a different model computer.

Another factor lies in the effort necessary to maintain the processor of a language, correcting the inevitable malfunctions which are found, and ensuring the availability of the corrections to the community of users of the language. It has largely fallen upon the manufacturers themselves to render this service, and they have preferred to concentrate their efforts on one or two languages which are important primarily to maintain the continuity of choices made for reasons which are now mostly historic.

Nor is the claim that programs are simply aggregates of algebraic statements, a few control statements, and perhaps some standard procedures for the input and output of data, entirely false. But it is just as misleading as the idea that a typewriter is operated by just looking for the letters on some buttons and then pushing them. Simplicity of use, and that the principles of use lie within the experience of the user to grasp are certainly important requisites. This is only the beginning; a disciplined sense of harmony and hierarchy are still required to gain the fullest benefits from computation.

In this section, I shall discuss the fate of four different approaches to bringing a higher organization to computation. These are, in order

FLT
MBLISP
CONVERT
REC

A. FLT (Fundamental Logic Translator) (16)

FLT was substantially begun at RIAS in 1957 by Philip Merryman, in an attempt to bring order into an ambitious molecular orbital program which

was eventually completed by R.K. Nesbet. Some chance remarks by Merryman at that time revived some memories of discussions of earlier years at Aberdeen Proving Ground on how a compiler "ought" to be designed, and thereby initiated my interest in computation. Eventually an FLT processor was prepared for the IBM 709 machine language, but by that time not only had my own views diverged considerably from Merryman's, but it became obvious that the processor would require many more capabilities (e.g., a formula translator) before it became practically useful.

There were two noteworthy attributes of FLT. One was that there should be operators which modified not only the contents of memory locations, but as well those which modified memory location pointers. Such was the way in which Merryman proposed to pass through data structures – packed matrices – in the intricate way needed for his calculations, alternating calculations affecting the data with calculations of where the data was to be found.

The second innovation was to index the operations by what he called their "coordinates", that is, stylized times of execution. Rather than to write a program by setting down each operator in the order in which it was to be executed, one systematically listed all the operands – data or addresses – and noted the conditions under which they were to be modified, and in what way. In practice these specifications tended to become rather cumbersome, especially when it was necessary to refer to compound "coordinates".

The resultant processor was decently short, actually compiled a few rather trivial test examples, and contained a few technically interesting programming features, such as a list-linked data block structure. But it was never destined to be very useful.

B. MBLISP (Martin-Baltimore LISP) (17)

The programming experience which I gained in writing FLT was actually put to use in creating a LISP interpreter. I had become aware of LISP through acquaintaince with some of John McCarthy's programming assistants, and the MIT Industrial Liason Program, and we had even used LISP 1 in a RIAS

summer institute rather successfully for a number of symbolic programs. A brief resumé of this institute was described in D-9. LISP documentation was nonexistent at that time, so that our understanding of LISP was rather empirical. In the light of the preparation of FLT, it seemed that writing a LISP interpreter would be a simple matter, and in fact the only way to gain an adequate understanding of the structure of LISP. Such was the case; MBLISP was planned for about a month, written in two weeks, more thoroughly debugged over the ensuing six months, and extended in various ways for several more years, and has served as a training medium for a considerable number of students.

LISP (List Processor) (18) was the invention of John McCarthy and an indeterminate number of his students at MIT, intended for the symbolic manipulation of list structures in a recursive fashion; from its inception it relied heavily upon such theoretical concepts as Church's lambda-calculus and Turing's concept of a universal machine. MBLISP differed from LISP in some picayune details; notably concerning the role of the empty list and consequently in the definition of the predicate ATOM; but also in the way that truthvalues were designated. The result was even less compilable than LISP itself, due to such innovations as a way to define a function with a variable number of arguments, or with quoted arguments.

The material upon which LISP operates is strings of letters which contain neither spaces nor parentheses called ATOMs, and strings involving balanced parentheses, ATOMS and possibly LISTs, which are called LISTs. Such a reentrant definition of LISTs means that from the outset they are defined recursively, with the consequence that it is natural to define all operations on lists recursively, exploiting the harmony between the definition of the operator and the list on which it operates.

There are five, and only five, primitive operations on lists. These comprise three functions and two predicates:

(CAR L)	the first element of the list L
(CDR L)	the list L with the first element removed
(CONS X L)	a list L to which X has been adjoined as the first element
(ATOM X)	False if X is a list, true otherwise
(EQ X Y)	True if X and Y are the same atom, or both are empty lists, false if one argument is empty or atomic and the other not, and undefined otherwise.

All other operations are supposed to be built up from these five,

recursively if necessary. The very elegant way in which this is done is to define a special kind of list, called a *form*. There are a certain number of primitive forms, together with rules for forming composite forms, again resulting in a recursive definition of forms. Finally there is a recipe, written as a form, telling how any form may be used to evaluate the function which is supposed to be associated with it. The recipe, usually given a name such as EVAL, is a universal form in the sense of a universal Turing machine. It can be employed to effect the calculation of the value of the function represented by any form whatsoever, given its argument, which ability extends to the universal form itself.

The definition of a form is as follows:

1. any ATOM is a form
2. If X, Y, and L are forms, then
   (CAR L)
   (CDR L)
   (CONS X L)
   (ATOM X)
   (EQ X Y) are all forms.
3. If L is whatsoever list or atom,
   (QUOTE L) is a form.
4. If PI and QI are all forms, I = 1, N, then
   (COND (P1 Q1) (P2 Q2) . . . (PN QN)) is a form
5. If V1, V2, . . . , Vn are atoms, E, and A1, A2, . . . , An are forms, then
   ((LAMBDA (V1 V2 . . . Vn) E) A1, A2 . . . An) is a form.
6. If E, A1, A2, . . . , An are all forms, then (E A1 A2 . . . An) is a form.

The universal form EVAL then tells how, given a form and suitable ATOMs or LISTs to be used as arguments, one is to calculate the value of the function associated with the form. Roughly speaking,

1. ATOMs are evaluated by looking up their values on a list which serves as a dictionary (which is formed in the process of evaluating a LAMBDA form, or possibly given initially).
2. The primitive function forms are evaluated by first evaluating their argument form or forms, and then performing the indicated operation.
3. The value of a quoted argument is that selfsame argument.

4. To evaluate a conditional form, one evaluates the first member of the first argument pair, P1. If it is true, one then evaluates the paired form Q1, whose value is taken as the value of the conditional form. If P1 is false, one repeats the process with the second argument pair and so on.
5. To evaluate a lambda-form, first evaluate any argument forms A1, A2, ... , An which may be present. They are then placed in the dictionary, associated with their corresponding variable names, V1, V2, . . . , Vn. Finally the form E is evaluated, its value becoming the value of the entire form.
6. In the remaining case the form E is evaluated, a new list created consisting of the value of E followed by the same arguments as before; and the resultant form evaluated.

One can extend LISP by extending the list of forms, and providing a more elaborate version of EVAL to evaluate them. There are also numerous undefined situations, for example when none of the predicates Pi is true in a conditional form, not to mention such items as how TRUE and FALSE are to be represented. Nevertheless, as above specified, LISP is a logically complete language, of no more nor less power than a universal Turing machine. In many ways it is much more aesthetically pleasant than a Turing machine, and can be so used in courses on automata and the theory of computation.

In practice, however, such a language is not usable. At the least, one has to be able to introduce definitions, and even synonymns, to allow a form to be given a single atomic name. In principle this may be accomplished by an introductory LAMBDA, and was also possible with a LABEL form which existed in McCarthy's original version, but the parenthesis nesting thereby incurred is not pleasant. Nor is such a technique one amenable to replacing a form by a machine language subroutine in the interests of greater efficiency, and without affecting the external appearance of any programs. The usual definition mechanisms are not easy to incorporate into the rules given above.

Graver problems beset the LISP user who wishes to use numbers, not to mention arrays, the data material of FORTRAN. Regrettably there has never been an adequate solution to the number representation problem in LISP, particularly as regards an efficient processor, competitive with FORTRAN. Notationally there are reasonably aesthetic ways to introduce

entities such as numerals, say as a specialized type of ATOM, but it is especially the electronic structure of most computers which frustrates the mixing of lists and arrays. Perhaps the most efficient of all such processors, prepared by Lowell Hawkinson and Robert Yates for the IBM 709, has never been circulated publicly.

LISP has had some use in Quantum Chemistry and High Energy Physics because it is possible to program such processes as symbolic differentiation, calculation of Poisson or commutator brackets, simplification or transformation of algebraic expressions, or calculating group tables, classes and irreducible representations of finite groups with a minimum of arithmetical capability.

C. CONVERT (D-10)

The language CONVERT came into being for two reasons; one general and one specific. The specific reason was that I had a series of calculations to make which involved the matching of lists to certain patterns, followed by a replacement of some of their parts. Symbolic differentiation is an excellent example of the aplication of such a process, wherein one has a series of rules for the differentiation of algebraic expressions. Rather than resorting to the definition of derivatives in terms of limits, one merely invokes the derivative rules recursively until he has differentiated his expression, however complicated. One of the intended aplications was the construction of tables of Poisson brackets, whose rules are substantially the same as those for differentiation.

The general motivation was the fact that the variable binding in LISP has to be accomplished using the LAMBDA-forms, whose use on a large scale or in complex situations is rather awkward. Not only do the word LAMBDA and several parentheses have to be written each time; the most cumbersome aspect notationally is the fact that the expression to be evaluated is sandwiched between the list of variables and the list of arguments. An excellent device for emphasizing a functional notation when the expression is short, its coherence is completely lost when the expression occupies several lines. After considerable experimentation, CONVERT was evolved as a pattern-directed language, somewhat after the style of COMIT (19), which

was also developed at MIT, by V. Yngve. However, CONVERT still held to the recursive style of LISP, and contained the distinctive feature for pattern matching languages that it was not only possible to specify that a variable should match a pattern, but also the exact conditions under which the match should take place.

CONVERT is defined in roughly the same manner as LISP. The data structures which it recognizes are atoms, fragments, and lists. Fragments are lists without confining parentheses. For practical purposes there eventually arises the need to include numbers and arrays as data types. Since these are somewhat artificial concepts occasioned by the desire to employ computer hardware efficiently, no thoroughly satisfactory syntax has ever been evolved for them.

There are two classes of forms in the CONVERT syntax, pattern forms and skeleton forms. Pattern forms, or simply patterns, are destined to be matched against lists, in order both to assert that a list has a certain structure, and to identify selected parts of the list. For example, with the variable X, the pattern (X * 0) could be used to decide whether a certain variable were multiplied by zero for purposes of algebraic simplification. Skeletons, on the other hand, are destined to have their variables replaced by values discovered during the matching process.

Primitive patterns consist of atoms, variables which have been given modal types, or recognizers of particular kinds of expressions such as atoms or numbers. Composite patterns can be formed, either as Boolean combinations of other patterns, or as lists. The Boolean "or" of several patterns, for example, means that if at least one of the patterns matches, the composite matches. The fact that alternatives are permitted and that it is possible to assign names to patterns permits the recursive definition of patterns. Lists match only if their CARs and CDRs separately match.

Primitive skeletons likewise consist of atoms or variables which have been given mode declarations, and presumably have acquired values during the matching process. Composite skeletons can be built up as lists, be built up recursively from the successive substitution of named skeletons, or can be control skeletons. Control skeletons permit the binding or freeing of variables as desired, followed by a new cycle of pattern matching and skeleton building, and are essential when several stages of matchings and substitutions are required to arrive at a final result.

Finally, a CONVERT program consists of a series of rule sets, a rule

being the pair (Pi Si) of a pattern Pi and a skeleton Si. Starting with the first pair of the set, we match its pattern to the expression to be converted. Should the pattern match, so that the necessary variables will have become defined, subsitution is made in the corresponding skeleton. If the pattern fails to match, the next pair is consulted and so on until a match is obtained. If all fail, the expression remains, unmodified. For each CONVERT program the variable patterns and skeletons which it employs have to be defined.

Although CONVERT is logically independent of LISP, and a universal CONVERT program can readily be written in the CONVERT language, so far the only processor constructed has been an interpreter written in LISP. CONVERT has been used for a number of unpublished group analyses and character tables, but with the decomissioning of the CeNaC's IBM 709, we have no longer had an adequate LISP to drive CONVERT. Moreover, the same deficiencies in number handling which negates LISP's usefulness are also found in CONVERT, although the CONVERT syntax accepts numbers slightly more readily than does LISP's. Until such time as a processor is constructed which is proficient in arithmetic, CONVERT will probably not receive widespread use.

An example of the use of CONVERT, and a comparison with SNOBOL, an outgrowth of COMIT, is found in D-11.

D. REC (Regular Expression Compiler) (D-12)

To deal with recursively defined data structures a processor which is itself recursive is extraordinarily convenient. Such data structures are typical of many symbol manipulation tasks, and indeed eminently typical of the task of compiler writing. Elsewhere, whether by tradition or by the inherent nature of the computation, it is much more convenient to use the iterative style of programming, which also corresponds much more closely to most computer hardware design. Recursive programming makes tremendous demands on the computer memory for the temporary storage of intermediate results, most of which are likely to be abandoned, unused, when the period of their retention has expired. Or, they are used in a way which could have been foreseen before the storage period began.

It is thus amusing that even for LISP, the epitome of recursive languages, its originators soon found it expedient to introduce a "program feature".

My objections are not so much to the use of the program feature as to the ad-hoc way in which it was introduced into LISP, effectively resulting in another language. The result of considerable reflection on this point was the concept of "operator predicates" which were introduced in one of the University of Florida program notes, and then eventually taken outside the framework of LISP altogether, to become the programming language REC.

One cannot say that REC operates on a particular kind of data structure, since it does not define the nature of its operators and predicates; these are supposed to be adequate in number and construction to treat their subject matter. It is only intended that the operators effect calculations and that in addition the predicates have a truth value. The REC language is then a scheme for combining the given operators so as to achieve a given sequence of calculations. For this organization REC uses four symbols of control. The parentheses, left and right, define a single expression, with the intention that an expression may be replaced at whatsoever moment by a single symbol if desired. The assignment of names and the unhindered freedom to use the name in place of the quantity named is fundamental to any orderly thought process.

Aside from the parentheses, a colon is used to signify that the expression is to be repeated from its beginning, while a semicolon is used to signify that its execution is terminated. In the language of regular expressions, then, a REC expression has the structure, where P is a predicate, Q an operator,

$$E = ([[P \vee Q \vee E]^{*} [; \vee :]^{*}]^{*} [P \vee Q \vee E]^{*})$$

To understand a regular expression one has to know that the square brackets are the usual mathematical sign of aggregation, v means an alternative between its arguments, * means the expression may be repeated a finite number of times, including zero, and that the symbols written in sequence are concatinated. One can give more formal definitions of regular expressions as well as REC expressions in terms of forms, with rules for interpreting the form as a function, just as was explained for LISP and CONVERT.

To execute a REC expression, one starts from the left parenthesis performing the operations called for by each operator, predicate, or REC expression, in the order in which they are written. After executing a predicate whose value is false one does not pass to the next sequential

expression, but rather to the expression first following the next colon or semicolon to the right of the predicate, in the same parenthesis level. If there is none, the execution of the regular expression terminates, and it is ascribed the value false. Thus a REC expression, taken as a unit, is itself a predicate.

If, in the course of executing a REC expression one encounters a colon, he then returns to the initial left parenthesis to continue operations, while if he encounters a semicolon, execution is terminated, and the entire expression is ascribed the value true.

A REC expression is therefore nothing but a program written in a very special way. Its characteristic features include:

1. subroutines, in the form of named REC expressions, may be used liberally. The processor must be written either so that *all* subroutines allow reentry or else it must be indicated as a part of the definition that a subroutine is to be recursive.
2. no labels are used in the program; only transfers to the beginning of the program or jumps over unexecuted segments are allowed, as required by the presence of colons, semicolons, or predicates.
3. the only exits allowed are to the end of the REC expression, either by a semicolon which ascribes the expression the value true, or arriving at the right parenthesis and ascribing the value false.

Such a restricted format clearly offers advantages and disadvantages. Experience has shown that the greatest molestation occurs when one has arrived at a certain point in a program as a result of a compound predicate, and does not know the exact cause. Boolean combinations of predicates are readily written. (P1; P2;) is the same as P1 *or* P2, (P1 P2;) is the same as P1 *and* P2, while (P;) is the same as *not* P. If P1 *and* P2 is false, it could be the result of the falsity of either P1 or of P2, so that if the distinction is important, a new test must be made. Other programming schemes might allow one to preserve this information at the time of the original test more conveniently than does REC.

Advantages of REC are that it is very concise, and that it conforms naturally to the thought processes in many programming situations.

Since nothing is said of a data structure, the burden is thrown completely on the programmer or preparer of the REC processor for a given application to ensure that his operators and predicates are capable of performing the necessary movements of data as well as effecting the

calculations desired. If a subroutine is to be recursive, explicit provision must be made for preserving any intermediate result which should not be destroyed. Nevertheless with sufficient freedom in making definitions, it is always possible to operate on such a level that such details do not become obtrusive. I have had considerable success in using a REC processor as a driver for complex FORTRAN subroutines, so that especially one does not suffer from the numerical inadequacies of LISP or CONVERT. Indeed my diminishing interest in either LISP or CONVERT stems from the possibility of securing all their advantages, when the time comes that they are desired, by setting up some appropriate REC subroutine.

REC has been used in a Hamiltonian Mechanics program, in a program for the numerical integration of the Schrödinger equation, in a matrix package used for teaching and casual calculations, and as an editor. There are being developed some programs for visual display on the PDP-15 (20), and some DDT versions for various DEC products.

V. QUANTUM MECHANICAL WAVE EQUATIONS

The material of this third section is very similar to that collected in the first part, with the important difference that it involves differential operators rather than matrices, and so is more a part of analysis than of algebra. This distinction is particularly manifest when it becomes apparent that the universal symmetry group which one would like to construct cannot exist more because of functions failing to satisfy boundary or integrability conditions than for the failure of algebraic identities which they should satisfy.

Reference D-21 is a detailed account of the search for symmetry and degeneracy in the two principal differential equations of quantum mechanics, the Schrödinger equation and the Dirac equation. The course of this search has been rather interesting. My interest in accidental degeneracy arose from learning about Schur's lemmas at about the same time as my graduate course in quantum mechanics. It was natural enough to suppose that the rotational symmetry of the harmonic oscillator and hydrogen atom accounted for their high degeneracy, and disconcerting to work things out and find that it didn't, after all. Fock's 1935 explanation (21) of the hyperspherical symmetry wasn't known around Ithaca, New York in 1950, and my first inkling that there was something interesting involved was a result of E.L. Hill's sending me, in 1954, a copy of his seminar notes (22) on the philosophy of quantum mechanics in exchange for some notes of my own. There were other intimations that strange things could be done with Schrödinger's equation – for example it was reputed that Schwinger, at Harvard, had a strange alchemy by which could be reduced all other problems to the harmonic oscillator.

Reference D-13 was an exposition of the results which I had managed to locate in the literature or work out on my own, up until 1958, and even yet it seems to be a respectable survey of that early period. However, the decade of the 60's saw a tremendous amount of activity, apparently touched off by Elliot's use (23) of Jauch and Hill's theory (24) of the accidental degeneracy of the harmonic oscillator in nuclear shell model calculations. At about the same time there was a realization that operators other than the symmetry operators could play a role in solving Schrödinger's equation. Operators such as the ladder operators which appeared in Schwinger's "Theory of Angular

Momentum" (25) could be used to raise and lower the total energy of the harmonic oscillator or the hydrogen atom. Infeld and Hull (26) had introduced ladder operators for differential equations in 1949, nevertheless there was a general feeling that they could be somehow better explained in the context of Lie Algebra. To the best of my knowledge, two articles by Goshen and Lipkin (27) constituted the first published use of operators obeying a definite commutation relation, but not commuting with the Hamiltonian, to obtain the shape as well as the degeneracy of the spectrum of the Hamiltonian.

By the mid 1960's two concepts had become quite well developed, that of a dynamical group and that of a universal symmetry group. The motivation was apparently the entymology of the numerous mesons and particles which had appeared in high-energy physics. The dynamical group is sometimes called the noninvariance group or the spectrum-generating group, names which clearly indicate its relation to the ideas of Goshen and Lipkin. Such groups existed, exactly for the hydrogen atom and the harmonic oscillator, because of the way in which Fock, and Jauch and Hill respectively had explained their accidental degeneracy. In both cases ample operators were available to construct much larger groups, and one only had to refrain from discarding those operators which *did not* commute with the respective Hamiltonians to have at his disposal ladder operators for the total energy. The whole spectrum, and not merely the degenerate states, could be generated at will.

The idea of a universal symmetry group arose from attempts to obtain the generators of dynamical groups in a systematic way, directly from the canonical commutation rules expressed in terms of Poisson brackets or matrix commutators. I had originally thought I had seen a way to obtain the canonical commutation rules from the standard form of the semisimple Lie Algebras, but the reverse turned out to be true – one can always construct an SU(n) group from the canonical commutation rules. Thus the articles D-14, D-15 and D-16 came into being, greatly aided by V.A. Dulock's discovery of a mapping between SU(3) and SO(4) which convinced many persons of the otherwise implausible claim that SU(3) was a symmetry group of the hydrogen atom, and also by his concoction of a felicitous expression which rendered the same service for the anisotropic harmonic oscillator – a result which Jauch and Hill had not succeeded in finding. As these were results in classical mechanics, they only intensified the

puzzlement concerning quantum mechanics, because we knew that the dimensions of the irreducible representations didn't coincide with the known degeneracies, to say the least.

It had always seemed desirable to have some other examples of accidental degeneracy besides the hydrogen atom and the harmonic oscillator, but Bertrand's theorem (28) rules out anything else with spherical symmetry and electrostatic forces in Euclidean spaces. Motion in a uniform magnetic field (D-15) was pretty much a variant on the anisotropic harmonic oscillator, although the regauging of the magnetic field (D-6) requires some precautions. M. Moshinsky had proposed a study of motion in the field of a magnetic dipole, on account of the interest of such things in Mexico City occasioned by Sandoval-Vallarta's cosmic ray investigations.

This was not satisfactory because so far the dipole problem has neither an analytic solution nor any evidence of accidental degeneracy, but motion in the field of a charged magnetic monopole is quite another matter, especially if it is endowed with an additional, albeit non-physical, centrifugal potential. It has SO(4) symmetry, as much so as the regular hydrogen atom, but with the interesting difference that different families of irreducible representations appear, depending upon the strength of the magnetic charge, which must be quantized to obtain a regular quantum mechanical problem. Because of the spherical, and not merely cylindrical, symmetry, gauge transformations enter in a non-trivial way and illustrate the angular-momentum-bearing qualities even of a static electromagnetic field.

The accidental degeneracy of the nonrelativistic magnetic monopole was investigated in D-20, written in collaboration with A. Cisneros, while the relativistic version and the Dirac equation appeared in D-18, written in collaboration with M. Berrondo. It was interesting to see that the symmetry and degeneracy of the hydrogen atom could be preserved even after the influence of the magnetic field of the monopole and relativistic corrections, in the manner of Biedenharn and Swamy's "symmetric" Dirac Hamiltonian (29). "Symmetric" Hamiltonians are interesting from a mathematical point of view since they exhibit the relation between accidental degeneracy and hidden symmetry in yet another context, but they lose some of their practical value because of the artificial potentials by which they differ from the "natural" Hamiltonians. Especially is the discrepancy severe in the Dirac equation for the charged magnetic monopole, where the natural Hamiltonian contains an attractive inverse square potential, which calls into play

an understanding of the basic principles underlying quantum mechanics. The difficulty is that it has never been decided how to quantize wave equations containing such potentials.

Mathematically the difficulty arises because of the boundary conditions which are to be imposed on the solutions. In most situations, which is to say when the potentials are not so singular, the requirement of square integrability with its associated probabilistic interpretation, adequately fixes a spectrum. When the potentials pertain to Weyl's so-called limit circle case, there exist mathematical procedures to select a spectrum and with it a complete orthonormal set of wave functions. In many cases, such as in the theory of angular momentum, a suitable boundary condition can be selected, but in others any selection whatsoever may be quite artificial. Especially, such is the case for the $1/r^2$ potential because it is dilationally covariant. The whole matter of singular potentials has been given a comprehensive review by Spector (30) but it requires much further investigation.

It would be interesting to know whether a monopole-antimonopole could combine to form a very long-lived composite. D-20 offered some hope, because the magnetic mirror effect tends to keep two charged monopoles from colliding unless they approach head-on. However, the symmetric monopole is more favorable to the separation than the natural monopole because the added centrifugal potential is repulsive. Unfortunately, for the Dirac equation matters become much worse because the orbital, field, and spin angular momentum can combine in a way that the fall to the origin is possible. For the ordinary Dirac equation, the spin and orbital angular momentum can nerver combine so as to permit the fall to the origin until atomic numbers greater than 137 are reached. Additionally the results of D-18 are inconclusive because they describe a single fermion moving around a boson nucleus. A relativistic two-particle equation, such as the Breit equation, or a Bethe-Salpeter equation, will compound the boundary value problems considerably, but should be examined so as to properly combine the spin, field, and angular momenta of both particles.

The usual manner of obtaining the SO(4) symmetry of the hydrogen atom is to use Fock's stereographic projection. Because none of the irreducible representations of SO(4) which arise from the Schrödinger equation of the monopole, the Dirac equation of the "symmetric" hydrogen atom or the Dirac equation for the symmetric charged monopole are

realizable as transformations defined on a hypersphere, a geometric explanation of their hidden symmetry cannot be made. The most systematic procedure which I have found to obtain the symmetry and degeneracy of the hydrogen atom and monopole problems is to separate the equations in parabolic coordinates. The Hamiltonian then resembles that of the harmonic oscillator sufficiently that, if the magnetic charge is taken as the conserved angular momentum conjugate to a cyclic coordinate, one can construct a unitary symmetry group and symplectic dynamical group using the recipies which have been given to construct the universal symmetry group. Some care is necessary, for it is possible to obtain slightly different dynamical groups, one of which operates only on the functional form of the wave functions, but does not scale the radius by the principal quantum number, 1/n, as the true dynamical group should. In both cases usable symmetry groups are obtainable. This was done with the false group for the two dimensional hydrogen atom in D-16, and for the true group in D-17. The more complicated three dimensional case has been very carefully worked out by J.L. Torres Hernandez in his professional thesis (31). When the constraint of conservation of magnetic charge is included, the preferred form of the dynamical group which is obtained is the SU(2,2) group of Malkin and Manko (32).

One of the principal motivations of the research leading to the papers of part III was my hope of finding some universally applicable principle, which would allow one to construct a symmetry group for whatsoever dynamical system. The early work of Jauch, Hill, and Saénz (33) unified the known "degenerate" systems – harmonic oscillator, hydrogen atom, and rigid rotor – in terms of force-free motion on a hypersphere according to the precedent established by Fock. The usefulness of this representation is rather definitively negated by the occurrence of the wrong representation in the spectrum of the symmetric monopole and Dirac equation, but from the outset I had thought that the use of ladder operators such as those of the harmonic oscillator would be a more likely approach. Finding SU(3) as a classical universal symmetry group was a bit much of a good thing since in quantum mechanics only one potential, that of the isotropic harmonic oscillator, seemed actually to possess such a symmetry group; and most potentials clearly had no degeneracy at all. Yet when several other authors announced the very same conclusion, some even including SO(4) as a universal symmetry group as well, the correctness of the result seemed indisputable.

Moreover the classical result was easy to accept, both because of work on adiabatic invariants, and because the main goal of classical mechanics course is always to show that "every problem can be reduced to force-free motion in a suitable space". But it was really careful attention to detail on the part of A. Cisneros in constructing the ladder operators and verifying their commutation relations that led to the results reported in D-19, perhaps the most important paper of the whole series. The universal symmetry group does not exist in quantum mechanics because it is not a group, and this because attention must be paid to the wave functions on which operators operate, to ensure that the formal solutions actually make sense. If an intermediate wave function is either put to zero or is not square integrable, it may invalidate a seemingly acceptable result gotten by formal algebraic manipulations.

Even though hopes for a universal symmetry group for Schrödinger's equation had to be abandoned, the ladder operators from which it was supposed to have been constructed are still available, and one is merely cautioned to use their commutation relations correctly. It is still an unresolved question as to whether any similar analysis is possible when the Schrödinger equation is not separable, and even in those cases where it might be possible to deduce the theoretical existence of the ladder operators it might not be practical to apply the recipe when it calls for ladder operators which are not simple rational functions of the coordinates and momenta. An adequate analysis of the hydrogen molecule ion, for example, could still yield considerable information about the occurrence of symmetry and degeneracy.

An exhaustive review of symmetry and degeneracy in the quantum mechanical wave equations according to the literature available and results various of my students and I had obtained up until the middle of 1968 is the content of reference D-21. Therein were surveyed all the potentials for both the Schrödinger equation and the Dirac equation, which had shown any degeneracy or which could merit attention for some related reason.

Aside from the information which they contain concerning specific potentials – for example the magnetic monopole – the principal merit which I claim for this third group of the publications is that they establish the very general possibility of using ladder operators constructed from the action-angle variables to explain the symmetry and degeneracy of the wave equations.

Contrary to the original expectations, these ladder operators do not always generate a group, which is why there is no universal symmetry group, or for that matter, no universal dynamical group. Occasionally, as in the replacement of SU(3) symmetry for the hydrogen atom by SO(4) symmetry, it is possible to obtain a group by some reorganization, and occassionally, as for certain harmonic oscillators with "excess angular momentum" one must accept that there is no possibility whatsoever of a group.

By their nature, their dependence on the action-angle variables, these ladder operators would seem to be still restricted to separable potentials. The reason for insisting on action-angle variables is, of course, that we need operators which satisfy the canonical commutation relations *and* are commutator-eigenfunctions of the Hamiltonian.

I have not offered such a wide selection of symmetry principles in part III for the wave equations as in part I for the matrix Hamiltonians. Indeed I would advocate abandoning the very technique on which the whole folklore of accidental degeneracy was founded – stereographic projections from hyperspheres – in favor of one single technique, based on the action-angle variable ladder operators. Even so, some of the algebraic principles enunciated in part I are helpful or even necessary when dealing with wave equations. To explain the accidental doubling in the Dirac equation for the natural hydrogen atom, Johnson and Lippman's anticommuting operator (34) plays the essential role.

There is one other area, very briefly hinted at in the final paragraph of reference D-8 which is beginning to receive some attention and deserves far more. By a judicious selection of the coordinate system and principal part of the Hamiltonian, the wave equation can be expanded in terms of a band-diagonal matrix, which may then be resolved by means of a recursion relation. Some degeneracies or non-degeneracies may be demonstrable in this form which are not apparent from the orignal wave equation. In particular, the results for the variation of a parameter are available, causing one to expect some rather sporadic degeneracies and level crossings, such as occur for the hydrogen molecule ion as its internuclear distance is varied.

There are still a few examples of symmetry and degeneracy in wave equations which have not yet found a place in my research, which hold promise of some interesting results. One is the cubical square well, with an infinite barrier. The solutions are purely plane waves, but due to the

quantization condition one obtains energies which depend upon the sums of squares of integers. Degeneracy is then an instance of Waring's problem, since we must know in how many ways a number may be written as a sum of squares. If a symmetry group were to be found besides, it would surely interest even number theorists.

There are Bethe-Salpeter equations in which higher groups, such as SO(4) occur. An adequate understanding of the problem of two monopoles will also surely require a Bethe-Salpeter equation. Both of these items should motivate a proper study of symmetry and degeneracy in the Bethe-Salpeter equations. Even the symmetry properties of the Dirac equation are still quite poorly understood. For example, one might ask for a potential wherein the degenerate doubling of levels does not occur. Numerical techniques will doubtless be of great assistance in such investigations. Anyone who feels that he can treat wave equations by purely algebraic manipulations, ignoring the boundary conditions, is probably not using the quantum mechanics which describes the real world. Much discussion of such matters as the correct quantization of angular momentum hinges upon this critical point, and as we have seen, this was just the undoing of the universal symmetry group. Finally there are cases such as the $1/r^2$ potential, superheavy Dirac point nuclei, and the charged monopole, in which it seems that perhaps Physics itself must have to be joggled a bit before it tells us which are the boundary conditions which Nature intended us to use.

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