The Racah–Wigner Algebra in Quantum Theory

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Section: Mathematics of Physics
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The Racah–Wigner Algebra in Quantum Theory

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Editor's Statement

A large body of mathematics consists of facts that can be presented and described much like any other natural phenomenon. These facts, at times explicitly brought out as theorems, at other times concealed within a proof, make up most of the applications of mathematics, and are the most likely to survive changes of style and of interest.

This ENCYCLOPEDIA will attempt to present the factual body of all mathematics. Clarity of exposition, accessibility to the non-specialist, and a thorough bibliography are required of each author. Volumes will appear in no particular order, but will be organized into sections, each one comprising a recognizable branch of present-day mathematics. Numbers of volumes and sections will be reconsidered as times and needs change.

It is hoped that this enterprise will make mathematics more widely used where it is needed, and more accessible in fields in which it can be applied but where it has not yet penetrated because of insufficient information.

GIAN-CARLO ROTA

Foreword

The study of the symmetries of physical systems remains one of the principal contemporary theoretical activities. These symmetries, which basically express the geometric structure of the physical system in question, must be clearly analyzed in order to understand the dynamical behavior of the system. The analysis of rotational symmetry, and the behavior of physical quantities under rotations, is the most common of such problems. Accordingly, every professional physicist must achieve a good working knowledge of the "theory of angular momentum."

In addition, the theory of angular momentum is the prototype of continuous symmetry groups of many types now found useful in the classification of the internal symmetries of elementary particle physics. Much of the intuition and mathematical apparatus developed in the theory of angular momentum can be transferred with little change to such research problems of current interest.

If there is a single essential book in the arsenal of the physicist, it is a good book on the theory of angular momentum. I have worn out several earlier texts on this subject and have spent much time checking signs and Clebsch-Gordan coefficients. Such books are the most borrowed and least often returned. I look forward to a long association with the present fine work.

A good book on the theory of angular momentum needs to be thoroughly reliable yet must develop the material with insight and good taste in order to lay bare the elegant texture of the subject. Originality should not be erected in opposition to current practices and conventions if the text is to be truly useful.

The present text, written by two well-known contributors to the field, satisfies all these criteria and more. Subtleties and scholarly comments are presented clearly yet unobtrusively. Moreover, the footnotes contain fascinating historical material of which I was previously unaware. The two chapters on the "theory of turns" and "boson calculus" are significant new additions to the pedagogical literature on angular momentum. Much of the theory of turns presented here was developed by the authors. By means of this approach the concept of "double group" is made very clear. The development of the boson calculus employs Gel'fand patterns in an essential way, in addition to the more traditional Young tableaux. This section provides an excellent prototype for the analysis of all compact groups.

The representation theory is developed in the complete detail required for physical applications. This exposition of the lore of rotation matrices is especially thorough, including the Euler angle parametrization as well as others of practical value.

The text ends with a long chapter on applications well chosen to illustrate the power of the general techniques. The book concludes with a masterly development of the group theoretical description of the spectra of spherical top molecules. To my mind the recent experimental confirmation of this theory in high resolution laser spectrometry experiments is one of the most spectacular confirmations of quantum theory.

The present text is really a book for physicists. Nevertheless, the theory generates substantial material of interest for mathematicians. Recent research (for example in non-Abelian gauge field theory) has produced topics of common interest to both mathematicians and physicists. Some of the more interesting mathematical outgrowths of the theory of angular momentum are developed in the companion volume currently in press.

PETER A. CARRUTHERS
General Editor, Section on Mathematics of Physics

Preface

"The art of doing mathematics," Hilbert[1] has said, "consists in finding that *special* case which contains all the germs of *generality*." In our view, angular momentum theory plays the role of that "special case," with symmetry—one of the most fruitful themes of modern mathematics and physics—as the "generality." We would only amend Hilbert's phrase to include physics as well as mathematics. In the Preface to the second edition of his famous book *Group Theory and its Applications to the quantum Mechanics of Atomic Spectra*, Wigner[2] records von Laue's view of how remarkable it is that "almost all the rules of [atomic] spectroscopy follow from the symmetry of the problem." The symmetry at issue is *rotational symmetry*, and the spectroscopic rules are those implied by *angular momentum conservation*. In this monograph, we have tried to expand on these themes.

The fact that this monograph is part of an encyclopedia imposes a responsibility that we have tried to take seriously. This responsibility is rather like that of a library. It has been said that a library must satisfy two disparate needs: One should find the book one is looking for, but one should also find books that one had no idea existed. We believe that much the same sort of thing is true of an encyclopedia, and we would be disappointed if the reader did not have both needs met in the present work. To accomplish this objective, we have found it necessary to split our monograph into two volumes, one dealing with the "standard" treatment of angular momentum theory and its applications, the other dealing in depth with the fundamental concepts of the subject and the interrelations of angular momentum theory with other areas of mathematics.

Fulfilling this responsibility further, we have made an effort to address readers who seek *very* detailed answers on *specific* points—hence, we have a large index, and many notes and appendices—as well as readers who seek an overview of the subject, especially a description of its unique and appealing aspects. This accounts for the uneven level of treatment which varies from chapter to chapter, or even within a chapter, quite unlike a

[1] Quoted in M. Kac, "Wiener and Integration in Function Spaces," *Bull. Amer. Math. Soc.* **72** (1966), p. 65. (The italics are in the original; Kac notes that the statement may be apocryphal.)

[2] E. P. Wigner, *Group Theory and Its Applications to the Quantum Mechanics of Atomic Spectra*, Academic Press, New York, 1959, p. v. (We have added in brackets the word "atomic," since this was clearly von Laue's intended meaning.)

textbook with its uniformly increasing levels of difficulty. The variation in the treatment applied particularly to the Remarks. Quite often these Remarks contain material that has not been developed or explained earlier. Such material is intended for the advanced reader, and it can be disregarded by others. We urge the reader to browse and skip, rather than trying, at first, any more systematic approach.

These considerations apply also to the applications. Some applications may be almost too elementary, whereas others are at the level of current research. The field of applications is so broad that we have surely failed to do justice in many cases, but we do hope that the treatment of some applications is successful.

In discussing a particular subject, we have given more detail than is usual in mathematical books, where terseness is considered the cardinal virtue. Here we have followed the precepts of Littlewood[3] who points out that "*two* trivialities omitted can add up to an *impasse*."

Let us acknowledge one idiosyncrasy of our treatment: We have not explicitly used the methods of group theory, per se, but have proceeded algebraically so that the group theory, if it appears at all, appears naturally as the treatment develops. No doubt this method of treatment is an overreaction to the censure—(now disappearing?)—with which many physicists greeted the *Gruppenpest*.[4] In any event, we think that this treatment does make the material more accessible to some readers.

Let us make some brief suggestions as to how to use the first volume, *Angular Momentum in Quantum Physics* (AMQP). Part I: (i) Chapters 2 and 3 and parts of Chapter 6 constitute the standard treatment of angular momentum theory and will suffice for many readers who wish to learn the mechanics of the subject. The methods used are elementary (but by no means imprecise), and the whole treatment flows from the fundamental commutation relations of angular momentum. (ii) Chapters 4 and 5 are recommended to the reader who wishes a general overview of the subject with methods capable of great generalization. Paradoxically, although these two chapters contain much new material, this material also belongs to the very beginnings of the subject—in the multiplication of forms of Clebsch and Gordan, and in the ξ-η calculus of Weyl—all of which are now incorporated under the rubric of the "boson calculus." Part II: The applications given in Chapter 7 are totally independent of one another, and can be understood from the results given in Chapter 3.

The second volume, *Racah–Wigner Algebra in Quantum Theory* (RWA), is also presented in two parts. (The Contents for RWA appears also at the

[3] J. E. Littlewood, *A Mathematician's Miscellany*, Methuen and Co., London, 1953, p. 30. (The italics are in the original.)

[4] B. G. Wybourne, "The Gruppenpest yesterday, today, and tomorrow," *International Journal of Quantum Chemistry*, Symposium No. 7 (1973), pp. 35–43.

beginning of AMQP.) Part I: In Chapters 2, 3, and 4 the algebra of the operators associated with the two basic quantities in angular momentum theory—the Wigner and Racah coefficients—is developed within the framework of the algebra of bounded operators acting in Hilbert space. These chapters are intended to rephrase the concept of a "Wigner operator" (tensor operator) in algebraic terms, using methods from Gel'fand's development of Banach algebras. This approach to angular momentum theory is rather new, and is intended for the reader who wishes to pursue the subject from the viewpoint of mathematics. Part II: The twelve topics developed in Chapter 5 establish diverse interrelations between concepts in angular momentum theory and other areas of mathematics. These topics are independent of one another, but do draw for their development on the material of Chapter 3 of AMQP, and to a lesser extent on Chapters 1–3 of RWA. This material should be of interest to both mathematicians and physicists.

Acknowledgments

This monograph could not have been completed without the extensive help of friends and colleagues. Professor L. P. Horwitz performed the vital chore of a thorough reading and criticism of the entire two volumes; his help is gratefully acknowledged.

Other colleagues who have helped us by reading and criticizing particular chapters, the applications, or topics in *Angular Momentum in Quantum Physics* and in *Racah–Wigner Algebra in Quantum Theory* are: (i) AMQP. D. Giebink, Chapters 2–4; Professors H. Bacry and B. Wolf, Chapter 4; Professor R. Rodenberg and Dr. M. Danos, Chapters 2–6; Professor B. R. Judd, Chapter 7, Section 5; Drs. H. W. Galbraith, C. W. Patterson, and B. J. Krohn, Chapter 7, Section 10; (ii) RWA. Professor L. Michel, Chapters 2–4; Drs. H. Ruch and R. Petry, Topic 2; Dr. M. M. Nieto, Professors M. Reed, N. Mukunda, and H. Bacry, Topic 7; Professor T. Regge, Topic 9; Dr. B. J. Krohn, Topic 10; Dr. C. W. Patterson and Professor J. Paldus, Topic 12. Dr. W. Holman read both volumes to assist us with the indexing and suggested many improvements. Further acknowledgment of help from those not mentioned here is indicated in the relevant chapters.

In a more general way, we are indebted also to Professors H. van Dam, E. Merzbacher, A. Bohm, and Dr. N. Metropolis for discussions and help extending over several years.

This monograph is dedicated to Professor Eugene P. Wigner, whose picture (courtesy of the Niels Bohr Library of the American Institute of Physics) appears as the frontispiece. We not only acknowledge the inspiration of Wigner's research, but also record his personal encouragement and help, and we are honored that he has accepted this dedication. We wish also to acknowledge our great indebtedness to the late Professor Giulio Racah, who encouraged our work at its most critical time, the very beginning. Professor Ugo Fano also helped us greatly in this same period.

Special thanks are due to Professor Gian-Carlo Rota, editor of this Encyclopedia, for encouraging us to write at length on the subject of this monograph.

Most monographs begin as course notes and lectures series. The present monograph is no exception and evolves from such notes and lectures given over the years. We are particularly indebted to Dr. H. William Koch for urging us to write up the lectures on angular momentum theory (based on the concept of the turn) given at the National Bureau of Standards. This was finally achieved many years later, when a much expanded version was presented at Canterbury University (Christchurch, New Zealand, in 1973) and supported by an Erskine Fellowship arranged by Professor Brian Wybourne.

Without the patience and helpful attitude of the editorial and production staffs of the Advanced Book Program of Addison-Wesley, and the free-lance copy editor, Dorothea Thorburn, it would not have been possible to split our original manuscript into the present two volumes.

The entire typing of the original manuscript and several of its revisions were carried through, courageously and without flinching, by Nancy Simon. Her loyalty to this task, extending over several years, is especially appreciated. Thanks are also given to Lena Diehl for typing many of the final revisions. We are also indebted to Graphic Arts and Illustration Services of the Los Alamos Scientific Laboratory for the figures and reproductions.

The writing of a monograph can be traumatic to others besides the authors. We wish to thank our wives, Sarah Biedenharn and Marge Louck, for their unfailing support and encouragement in keeping us at our task.

L. C. BIEDENHARN
J. D. LOUCK

Introduction

1. This book is a sequel to its authors' recently published *Angular momentum in quantum physics*: *Theory and application*; it treats various advanced topics that could not be covered in the earlier volume without making it inconveniently long. My purpose is to explain the subject matter from a mathematician's point of view, but it would be awkward and difficult to do this without taking into account the contents of both books. Thus, in spite of its tardy appearance, this essay will, in effect, be an introduction to the two-volume work as a whole.

When a physicist speaks of "angular momentum theory," he is alluding to a theory that a mathematician would be more likely to describe as "the theory of rotational invariance." This theory, whatever we call it, is concerned (*a*) with a technique for exploiting the fact that many physical laws are independent of orientation in space and (*b*) with the many important consequences of this fact.

The physicists' choice of the words "angular momentum theory" illustrates a tendency that is one of the many factors inhibiting communication between mathematicians and physicists. This is the tendency physicists have to avoid thinking in the abstract and instead to keep a concrete physical problem constantly in mind and use physical terminology whenever possible. From the mathematician's point of view, the physicist is behaving like a beginner who will not take the step from "two oranges and two oranges is four oranges" to "two plus two equals four." The physicist is much less practiced in abstract thinking and is quite properly reluctant to give up an important source of intuition and inspiration.

But what is the connection between rotational invariance and angular momentum that inspires this terminology? It derives from a fundamental

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theorem in mechanics—both classical and quantum—setting up a natural one-to-one correspondence between certain "one-parameter symmetry groups" on the one hand, and "integrals of the motion" on the other. The group $\mathfrak{S}$ of all rigid motions of Euclidean space defines an action of $\mathfrak{S}$ on the phase space Ω of an n-particle system, and for each x in $\mathfrak{S}$ the associated one-to-one map of Ω on Ω is a "symmetry" of the system in an obvious sense. If $s \rightarrow \alpha_s$ is any one-parameter subgroup of $\mathfrak{S}$—that is, any continuous homomorphism of the additive group of the real line into $\mathfrak{S}$—then this homomorphism composed with the action of $\mathfrak{S}$ defines an action of the real line on Ω, each map of which is a symmetry. Thus, one has an integral of the motion that is, a function on Ω that is constant in time) for each one-parameter subgroup α of $\mathfrak{S}$. These integrals, which are evidently of special interest, are called momentum integrals. Given a line l in space, let α_s^l denote the rotation about l through an angle of s radians. The integral of the motion corresponding to this one-parameter symmetry group is called the *total angular momentum* about the axis l. Linear momentum is defined similarly, with one-parameter groups of translations. Although the linear and angular momentum integrals were discovered long before anyone thought in terms of groups of symmetries, it is gratifying to have such an elegant a priori reason for their existence.

2. Before proceeding further, it will be useful to recall the basic structure of quantum mechanics in the rigorous form given it by von Neumann. This can be done quite concisely and completely, and a reader unfamiliar with quantum mechanics (at least in this formulation) should not hesitate to make a serious effort to understand it.

In classical mechanics the future of a system of n particles in uniquely determined by the positions and velocities of these particles at any instant of time t. The $6n$-dimensional space Ω of all possible positions and velocities of the particles is called the *phase space* of the system, and its points ω are called the *states* of the system. (For reasons that need not concern us, one actually uses positions and momenta; the momentum of a particle being the mass times its velocity.) For each positive real number t and each $\omega \in \Omega$, let $\alpha_t(\omega)$ denote that point ω' of Ω such that the positions and velocities corresponding to ω' are precisely those that describe the system t time units after it was described by the positions and velocities corresponding to ω. Then in all "reversible" systems (and we consider no others), each α_t is a one-to-one map of Ω on Ω, and setting $\alpha_{-t} = \alpha_t^{-1}$ we obtain a one-parameter group $t \rightarrow \alpha_t$ of one-to-one transformations of Ω into itself. Let us call this the *dynamical group* of the system. The parameterized curves $t \rightarrow \alpha_t(\omega)$ are the *trajectories* of the system, and we obtain a vector field X^α in Ω by assigning to each point ω the tangent vector to the unique trajectory through ω. This vector field is called the *infinitesimal generator* of the dynamical group α, and via uniqueness theorems for systems of ordinary differential equations it determines α uniquely. The unique determination of α by X^α is of the greatest importance for physics, because in most cases X^α can be written down explicitly, whereas α cannot. Thus, nontrivial mathematical problems remain to be solved after the physical law has been precisely formulated. Real valued functions on Ω—that is, functions of the coordinates and velocities—are called *observables* or *dynamical variables*. If f is an observable and $\omega \in \Omega$, then $f(\omega)$ is said to be the *value of the observable* in *the state defined by* ω. Since ω varies with time, the value of any observable f will also vary with time according to the formula $t \to f(\alpha_t(\omega))$. However, there are certain observables g that are such that $t \to g(\alpha_t(\omega))$ is a constant for all ω. These are called *integrals of the motion*, and they are precisely those functions g on Ω that are constants on the trajectories.

In quantum mechanics the states (points of Ω) are replaced by the one-dimensional subspaces of a separable complex Hilbert space $\mathcal{H}$, and the dynamical group is replaced by a continuous one-parameter group $t \to V_t$ of unitary operators mapping $\mathcal{H}$ onto $\mathcal{H}$. By a celebrated theorem of M. H. Stone (inspired by the needs of quantum mechanics), every one-parameter unitary group $t \to V_t$ may be put uniquely in the form $V_t = e^{iHt}$, where H is a (not necessarily bounded) self-adjoint operator. This operator H is the analog of the vector field X^α in classical mechanics and is what one can write down explicitly. If ϕ is a unit vector in the one-dimensional subspace specifying a state at time 0, then this state will be specified t time units later by the one-dimensional subspace containing $V_t(\phi)$, and the variable vector $t \to V_t(\phi) = \phi_t$ will satisfy the differential equation $d\phi_t/dt = iH(\phi_t)$. This (in abstract form) is the Schrödinger equation—the quantum mechanical substitute for the equations of motion of a classical mechanical system. Just as in classical mechanics, the state of a system at a future time t is uniquely determined by t and the state at time 0.

The key difference between quantum mechanics and classical mechanics lies in the fact that the number $f(\omega)$, which the state defined by ω assigns to the observable f, is replaced in quantum mechanics by a probability distribution. In every quantum mechanical state there will be observables that do not have a well-determined value. If one makes the appropriate measurements, one gets different values, but some occur much more frequently than others, and one does have a well-defined probability measure on the line. Our task now is to explain how to calculate the probability distribution of an observable $\mathcal{O}$ in a state s when we know the self-adjoint operator A defining $\mathcal{O}$ and the one-dimensional subspace L of $\mathcal{H}$ defining s. This will be the quantum mechanical substitute for $f(\omega)$. The task is quite trivial when the operator A has a pure point spectrum—that is, when $\mathcal{H}$ admits an orthonormal basis $\phi_1, \phi_2, \ldots$ such that $A(\phi_j) = \lambda_j \phi_j$ for $j = 1, 2, \ldots$. Let ψ be any unit vector in L. Then $\psi = \sum_{j=1}^{\infty} c_j \phi_j$, where $c_j = (\psi \cdot \phi_j)$ and

$\sum_{j=1}^{\infty} |c_j|^2 = 1$. Also, $|c_j|$ is independent of the choice of ψ in L. Setting $\mu_L(E) = \sum_{\lambda_j \in E} |c_j|^2$, we obtain a probability measure on the real line, and this is the probability measure assigned to the observable $\mathcal{O}$ defined by A when the system is in the state s defined by L. Note that the probability that the measurement of $\mathcal{O}$ is not one of the eigenvalues λ_j of the operator A is zero. Of course, self-adjoint operators may have continuous spectra, and then the associated probability measures will not be concentrated in countable sets—not all quantum mechanical observables are "quantized." To compute μ_L when A has a (partially or totally) continuous spectrum, it is necessary to resort to the spectral theorem. We shall not attempt to explain the spectral theory here. Readers who are familiar with the theorem will have no difficulty in adapting the above.

Although it is necessary to diagonalize A in order to compute the probability distribution of the corresponding $\mathcal{O}$ in the various states, the "expected value" of $\mathcal{O}$ can be computed directly from A and ψ. When A has a pure point spectrum so that $\mu_L(E) = \sum_{\lambda_j \in E} |c_j|^2$, it follows at once from the definition that the expected value of $\mathcal{O}$ is $\sum_{j=1}^{\infty} \lambda_j |c_j|^2$. On the other hand, if $\psi = \sum_{j=1}^{\infty} c_j \phi_j$, then

$$A(\psi) = \sum_{j=1}^{\infty} c_j A(\phi_j) = \sum_{j=1}^{\infty} c_j \lambda_j \phi_j,$$

so

$$(A(\psi)\cdot\psi) = \sum_{j=1}^{\infty} c_j \overline{c_s} \lambda_j (\phi_j \cdot \phi_j) = \sum_{j=1}^{\infty} \lambda_j |c_j|^2.$$

Thus, the expected value is just $(A(\psi)\cdot\psi)$. This result can be shown to hold even where A does not have a pure point spectrum.

Finally, let A be the self-adjoint operator defining an observable $\mathcal{O}$. Under what conditions on A shall we say that $\mathcal{O}$ is an "integral of the motion"? In classical mechanics we required that $f(\alpha_t(\omega))$ be independent of t for every ω in Ω. The obvious analog is that the probability distribution defined by A and $V_t(\psi)$ be independent of t for every unit vector ψ. This is equivalent to demanding that the probability distribution defined by $V_t A V_t^{-1}$ and ψ be independent of t for every unit vector ψ. This can be shown to happen if and only if $V_t A V_t^{-1}$ is independent of t—that is, if and only if A commutes with all V_t. Accordingly, an integral of the motion in quantum mechanics is an observable whose corresponding self-adjoint operator A commutes with all V_t. Recall that $V_t = e^{iHt}$ for some self-adjoint operator H. Evidently the observable corresponding to H is an integral of the motion and, moreover, one that plays a special role. It is a constant multiple of the quantum mechanical analog of the energy integral of classical mechanics. Note that the state defined by the unit vector ψ will be stationary—that is, independent of the time—if and only if $V_t(\psi) = e^{i\lambda t}\psi$ for some real λ and all t. On the other hand, it is easy to see that $V_t(\psi) = e^{i\lambda t}\psi$ if and only if $H(\psi) = \lambda\psi$. Thus, the stationary states are precisely the states in which the energy observable has a definite value with probability 1, the possible values being constant multiples of the eigenvalues of H. As will be explained more fully below, this fact is the key to the quantum mechanical explanation of atomic spectra. In particular, it largely reduces the problem of predicting spectral lines to finding the eigenvalues of certain self-adjoint operators.

3. With the abstract structure of quantum mechanics before us, it is possible to explain the correspondence between one-parameter symmetry groups and integrals of the motion alluded to in section 1. By definition, a symmetry of a quantum mechanical system is a pair α, β consisting of a one-to-one mapping α of the states on the states and a one-to-one mapping β of the observables on the observables such that the following two conditions are satisfied:

*For all states s and all observables $\mathcal{O}$, the probability measure in the line assigned to $\beta(\mathcal{O})$ by $\alpha(s)$ is the same as that assigned to $\mathcal{O}$ by s.

**For all states s and all real numbers t, $\tilde{V}_t(\alpha(s)) = \alpha(\tilde{V}_t(s))$, where $\tilde{V}_t$ is the map of states into states defined by the unitary operator V_t.

It is a theorem that any pair α, β that satisfies (*) is defined by an operator U that is either unitary or anti-unitary. If s corresponds to the one-dimensional subspace L, and $\mathcal{O}$ to the self-adjoint operator A, then $\alpha(s)$ corresponds to $U(L)$, and $\beta(\mathcal{O})$ to UAU^{-1}. The operator U is uniquely determined up to multiplication by a complex number of modulus 1. In order that (**) should also be satisfied, it is evidently necessary and sufficient that for each real t we have $UV_tU^{-1} = c(t)V_t$, where $c(t)$ is a complex number of modulus 1. Since the square of an anti-unitary operator is always unitary, an obvious argument shows that only unitary operators occur in one-parameter symmetry groups. A less easy argument allows one to eliminate the constant $c(s_1, s_2)$ in $U_{s_1+s_2} = U_{s_1}U_{s_2}c(s_1, s_2)$ and to show that every one-parameter symmetry group is implemented by a one-parameter unitary group $s \to U_s$. By Stone's theorem, $U_s = e^{iAs}$ for some self-adjoint operator A. The operator A is determined by the symmetry group up to an additive constant. Condition (**) is satisfied if and only if $U_sV_t = c(s, t)V_tU_s$