

# Symmetry and Degeneracy\*

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Throughout this article we shall be describing wave equations, both Schrödinger's and Dirac's for a wide variety of potentials. The notation for the parameters appearing in these equations, their eigenvalues and eigenfunctions is now well standardized and nearly universal, and we shall frequently refer to them by name, without further ceremony; for example, the magnetic quantum number  $m$ . Furthermore, we shall take  $\hbar = c = 1$ , as well as taking 1 for a particle's mass, except that we will retain an explicit  $m$  in relativistic formulas.

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# I Introduction

Ten years ago it was possible to summarize the subject of accidental degeneracy in a somewhat lengthy personal letter, which was published (1) in the *American Journal of Physics* after slight adaptation. Ten years ago, accidental degeneracy was still a somewhat esoteric subject, pursued by those who wondered about the real reason for all the degeneracy in the hydrogen atom or harmonic oscillator, but still considered not quite suitable for a major research effort. With the passage of a decade, the outlook has changed greatly; just as the volume of published literature has grown enormously. In the main, two developments are responsible for this evolution. First of all, it was found that in nuclear theory, the near identity of results obtainable with the collective model of the nucleus and the independent particle model could be attributed to the assumption of a harmonic oscillator potential in the absence of definite knowledge of nuclear forces. The constants of the motion belonging to the harmonic oscillator resulted in strong correlation of the motion of ostensibly independent particles, and one could build up reasonable nuclear wave functions from states degenerate in the harmonic oscillator potential. The group responsible for the degeneracy is the unitary unimodular group  $SU(3)$ , and not the smaller three dimensional rotation group which expresses the obvious spherical symmetry of the harmonic oscillator Hamiltonian.

Second, the success of  $SU(3)$  in dealing with nuclear problems was followed by considerable progress in classifying the properties of elementary particles according to the irreducible representations of various Lie groups, among them  $SU(2)$ . Attempts to extend these results or to place them on a sounder footing are directly responsible for this renewed interest in the whole area of symmetry, degeneracy, and accidental degeneracy. In part there is a hope that what worked for nuclear theory will somehow work out for elementary particle theory as well. But, there is also a more systematic basis for such studies, arising from the fact that a great part of the advances in quantum electrodynamics in the late forties was due to the careful adherence to relativistic invariance in describing physical phenomena. It could be argued that the Lorentz group may not be the most general possible group, some evidence existing, for example, that physical laws should be invariant under the conformal group. One step in the right direction toward establishing the existence of such a group would be to obtain a better understanding of the symmetry of some common physical systems.

Quite aside from speculations as to whether general relativity or some other philosophical innovation should modify our position regarding symmetry principles applicable to all physical systems, there has been mounting evidence that our understanding of contemporary quantum mechanics is not as clear and well defined as it ought to be. It is not that a precise and axiomatic foundation is lacking so much as the fact that most of the familiar usage of quantum mechanics occurs in contexts and for applications in which the most careful formulation is not required. For example, one rarely encounters singular potentials for which the simple requirement of square integrability of the wave function is not sufficient to achieve quantization. But again, recent work points to the prevalence of singular potentials, and even to some related niceties which make themselves felt when familiar systems are treated in unfamiliar coordinate systems.

Whatever might have been the reason for the activity of the past decade, there is now a much larger body of literature to survey, and a considerably clearer picture of symmetry in all branches of Hamiltonian mechanics, both classical and quantum mechanical, relativistic and nonrelativistic. Indeed, a complete survey would itself be quite voluminous, causing us to

confine the present article to a survey of what we might describe as symmetry and degeneracy in the single particle realm. Thus we make no attempt to discuss any of the field theories; we shall as well pass over interesting aspects of solid state and molecular and atomic physics. On the other hand, we shall try to set the single particle theory in as general a perspective as possible.

Before one can appreciate the interest in “accidental” degeneracy and “hidden” symmetry, it is helpful to meditate for a moment on symmetry of the more overt, readily apparent variety, and the importance and applications in physics and chemistry of these concepts. A great part of the activity of contemporary theoretical physics or theoretical chemistry reduces in the end to the diagonalization of matrices. There are a variety of reasons for this emphasis on linear operators, but the most important is perhaps that the basic equation: of these branches of science is the Schrödinger equation or its relativistic generalization, the Dirac equation. The basic philosophy of quantum mechanics is that all physically observable quantities are to be obtained from the eigenvalue problem for a suitable Hamiltonian. Even in more classical realms, eigenvalue problems occur in the treatments of small vibration problems, which form a realistic first approximation even to inherently much more difficult problems.

While adequate numerical methods exist for the task of matrix diagonalization, they are difficult to apply to very large matrices, larger than order 50 or 100, and in any event numerical methods do not often give as much theoretical insight into problems as do symbolic methods, not to mention that we may even often be dealing with finite-dimensional approximations to linear operators on infinite-dimensional spaces. Whatever methods might be available for separating a problem into simpler constituents are extremely valuable and have always been earnestly sought.

The exploitation of symmetry through group theoretical methods is one of the oldest of such techniques, and was introduced almost as soon as the operational methods of the “new” quantum mechanics made its application relevant. In the beginning, for example, an analysis of the permutational symmetry of the system was an almost indispensable part of the discussion of any many body problem, before Slater’s introduction of the determinantal wave functions. Spherical symmetry, with its relation to the conservation of angular momentum, has been essential to the understanding of atomic and molecular spectra, and even such rudimentary symmetries as those arising from time reversal and spatial reflections have had considerable influence in analyzing a wide variety of physical phenomena.

By and large, there has been no difficulty in exploiting ostensible geometric symmetry, which is manifested by a group of linear operators commuting with the Hamiltonian of the system. Schur’s lemmas describe the limitations imposed on the Hamiltonian, which are substantially that there be no matrix elements connecting wave functions of different symmetry types, and that all the eigenvalues belonging to one irreducible representation of the symmetry group be equal. This last mentioned requirement is, of course, the well-known relationship between symmetry and degeneracy. Every symmetric system will show characteristic degeneracies, whose multiplicity is prescribed by the dimensions of the irreducible representations of its symmetry group. Yet, there is no restriction arising from group theoretical reasoning which prevents there from being a higher multiplicity of degeneracy than that required by Schur’s lemmas, but any degeneracy so arising is commonly called “accidental” degeneracy due to a presumption as to its unlikelihood.

Over the years there has been continual progress in finding methods suitable for the computation of symmetry-adapted functions belonging to a variety of groups. Once the symmetry-

adapted functions are found, the Hamiltonian may be partially diagonalized with the result that the determination of the secular equation, as well as of its eigenvalues and eigenfunctions, may be greatly simplified. In this way group theoretical methods are of considerable practical use, since they allow the reduction in the size of matrices which must be handled; a substantial saving since the amount of calculation required grows as the cube of the dimension of the matrix. Their theoretical importance is no less, for they may be used to justify rigorously the resolution of a complex system into a series of simpler noninteracting systems according to their symmetry type. Sometimes symmetry methods are better known in many-particle applications, where they are not introduced until some such simplifying separations have already been made tacitly, paving the way for the subsequent introduction of a finite symmetry group. Crystal field theory or the Hückel approximation are good examples.

In practice a highly intriguing situation has been noticed. For a great number of the highly idealized and supposedly fundamental systems there has always been far more degeneracy present than was required by the geometrical symmetry group and Schur's lemma. For the most part the ostensible symmetry has been the spherical symmetry of the central forces in ordinary three-dimensional space, which has been known to require nothing more than a degeneracy in the  $z$  component of the angular momentum of the wave functions of those systems. The three most typical and extensively treated systems, the hydrogen atom, the harmonic oscillator, and the spherical top, also exhibit degeneracy for various additional combinations of quantum numbers, resulting in a degeneracy which is truly accidental in the context of spherical symmetry. Inasmuch as the hydrogen atom involves the Coulombic potential which is the universal potential of electrostatic interaction between point charges, the harmonic oscillator describes the first degree of approximation to the small vibrations of quite general systems about their equilibrium configurations, and an equally widespread approximation is to treat only the motion of the center of mass of a body and its rotation as though it were rigid, the simultaneous occurrence of degeneracy in the Schrödinger equations of three such disparate systems has escaped neither notice nor attempts to attribute to it a deeper significance.

There has always been a feeling that accidental degeneracy might not be so much of an accident after all, in the sense that there might actually have been a larger group which would incorporate several different degenerate representations of the overt symmetry group in a single one of its own irreducible representations. In a formal sense this is clearly true, for one can simply postulate the group of all operators commuting with a given Hamiltonian. This is a rather unacceptable resolution of the problem, because there may be no effective way of identifying the totality of such operators with symmetry operations or with some other quantity having physical significance. This is particularly true for the problems of single particle mechanics, in which one expects there to be a constant of the motion generating every infinitesimal canonical transformation.

Although linear operators, their symmetry groups, and degeneracies are the proper province of quantum mechanics, in any discussion of constants of the motion and canonical transformations, classical mechanics will quickly enter the scene, if for no other reason than the fact that most of the concepts and results which are valid in classical mechanics have a fairly immediate transcription into quantum mechanics. Here it must be remembered that historically symmetry has played an important role in classical mechanics as well, although mostly through the use of continuous groups of transformations, rather than their matrix representations. Again the basic concept is that of a canonical transformation -a transformation of the

phase space variables which leaves unchanged the Hamiltonian form of the equations of motion. Among the totality of such transformations there are those which leave the Hamiltonian itself unchanged. The preservation of the Hamiltonian is manifested in two ways: on the one hand, its functional form remains intact after the substitution of the new variables; on the other, when the canonical transformation is an infinitesimal transformation it may be thought of as the generator of a one-parameter Lie group of transformations. This parameter defines an orbit, consisting of the displacement of the point for varying values of the parameter. For example, the  $z$  component of angular momentum generates, about the  $z$  axis, rotations whose orbits are circles orthogonal to and centered on the  $z$  axis; the square of the angular momentum generates, about the angular momentum vectors, rotations which rotate each point in its own plane of motion, which is orthogonal to its angular momentum vector.

Such is our understanding of a symmetry generated by a constant of the motion; the analytic test for such a constant, when it contains no functional dependence on the time, is that its Poisson bracket with the Hamiltonian be zero. However, this is a mutual relationship and inasmuch as the same Poisson bracket describes the temporal variation of the generator, one concludes that this variation must also be zero. Hence, the generators of a symmetry group for the Hamiltonian are also constants of the motion. Rather similar considerations apply to quantum mechanical operators.

The requirement then is for a “hidden” symmetry: a symmetry not necessarily of a geometric nature, but which together with the geometric symmetries already known would yield a group large enough that its irreducible representations would account for exactly all the observed degeneracies of the system. Classical Hamiltonian mechanics actually contains a reasonable source of hidden symmetries because it deals with a phase space of double the dimension of the configuration space in which the geometric symmetries are evident. In other words, it might be entirely possible that there are additional symmetries of the phase space as a whole which would comprise the desired group.

## II Symmetry of the Hydrogen Atom

Fock’s paper of 1935, *Zür Theorie des Wasserstoffatoms* (2), was something of a landmark in this respect, wherein it was shown that just such an explanation could be given for the degeneracies of the hydrogen atom. As a central force problem, the hydrogen atom possesses spherical symmetry. Nevertheless spherical symmetry is only adequate to account for degeneracy in the magnetic quantum number  $m$ , while the energy of the hydrogenic levels depends only on the principal quantum number  $n$ , and is independent of the value of the quantum number of the total angular momentum, which may range from 0 to  $n - 1$ . The result is that there is an  $n^2$ -fold degeneracy for the principal quantum number  $n$  rather than a  $(2\ell + 1)$ -fold degeneracy for the angular momentum quantum number  $\ell$ .

Such a quantum mechanical degeneracy was reminiscent of a well-known classical degeneracy in the corresponding problem of planetary motion, for it was recognized that the energy of the orbit in Keplerian motion depended only on the semimajor axis of the trajectory, which was always a planar conic section, and not upon its eccentricity. The planarity of the orbit was an established consequence of the conservation of angular momentum, and therefore due to the spherical symmetry of the inverse square Newtonian attraction. However, the orbits of the Kepler problem are almost unique among all the central force problems in that the bounded

orbits are simple closed curves, for it seems that only the orbits of the harmonic oscillator share this property. In general such orbits are space filling, a result which was demonstrated by Bertrand almost a century ago. Thus even in classical mechanics the inverse-square force law manifests some exceptional characteristics.

The Hamiltonian for the hydrogen atom is

$$\mathcal{H} = \frac{1}{2}p^2 + V(r),$$

where

$$V(r) = -1/r.$$

Fock's demonstration depended upon writing its Schrödinger equation in a momentum representation, as an integral rather than a differential equation

$$\frac{1}{2}p^2\psi(p) - \frac{1}{2\pi^2} \int \frac{\psi(p')(dp')}{|p-p'|^2} = E\psi(p).$$

In this form, the kernel can be recognized as the Jacobian determinant for a stereographic projection from the surface of a four-dimensional sphere to three dimensions, which in turn suggests writing the Schrödinger equation in terms of angular variables on the hyperspherical surface, all of which finally results in an integral equation which may be recognized as the Poisson kernel for a hyperspherical surface harmonic in the degenerate case in which the field point has fallen onto the surface.

By thus placing the hydrogen atom wave functions clearly in evidence as hyperspherical surface harmonics, no doubt is left that the appropriate symmetry group of the hydrogen atom is the four-dimensional rotation group, and not merely the three-dimensional rotation group of the central forces. Strictly speaking one ought to distinguish three cases, according to whether the energy is positive, zero, or negative. The radius of the hypersphere from which the projection is made depends upon the reciprocal of the square root of the negative of the energy, so that only the bound states correspond to an actual hypersphere. In the other cases one deals with either a hyperplane, or the surface of a hyperboloid, so that in those cases the appropriate symmetry group is either an Euclidean group or a Lorentz group.

Immediately after the publication of Fock's paper, Bargmann (3), showed that the generators of the infinitesimal rotations of Fock's hypersphere were nothing other than the components of the angular momentum, together with the components of the Runge vector, when written in terms of the Cartesian components in ordinary three-dimensional space, and their associated conjugate momenta. The components of the angular momentum vector generate the rotations corresponding to the spherical symmetry of the Coulomb potential, so that the additional symmetry present, together with its degeneracy, is seen to be a consequence of the constancy of the Runge vector.

In point of fact, the Runge vector,

$$\mathbf{A} = \mathbf{L} \times \mathbf{p} + \hat{\mathbf{r}},$$

where  $\hat{\mathbf{r}} = \mathbf{r}/r$  in a unit vector in the radial direction, had been known, under various names, as a constant of Keplerian motion nearly from the time of Newton's original formulation of the law of universal gravitation and the description of the motion of heavenly bodies in terms of the calculus. Perhaps we should more aptly say, it has been known since the time of the

origin of such concepts as the vector calculus, which came somewhat after the invention of the calculus itself, by perhaps half a century. The Runge vector is a vector pointing to the perihelion of the orbit, whose magnitude is the eccentricity of the orbit. It is therefore an analytic token of the fact that the orbits for the inverse square law do not precess; for other force laws the orbit is typically some sort of rosette.

The earliest published reference to a vector such as the Runge vector which we have been able to find, and which was obviously the precursor of Runge's popular tract on vector analysis, is an article of Hamilton (4) of 1847, communicating a result presented before the Royal Irish Academy in 1845, in which quaternion notation was used to solve the equations of Keplerian motion, and the Runge vector is introduced as a quaternion with zero time derivative. In reality, of course, the fact that we are dealing with an elliptical orbit whose semimajor axis is fixed and which passes through the attracting center which is located at the focus goes back to the observations of Kepler. Nevertheless, we can only begin to touch upon such quantitative aspects as the vector transformation rules or the independence of the orbital energy from the eccentricity, after such mathematical concepts have been appropriately formulated.

Implicit in Hamilton's work are other aspects of the contemporary theory of the symmetry of the hydrogen atom. For example, he formulated the "law of the circular hodograph" which states that the hodograph of the Keplerian motion, uniquely among all force laws, is circular. By hodograph is meant the figure resulting from plotting all the velocity vectors of the motion from a common origin. The radius of the hodograph depends on the absolute value of angular momentum, while its plane depends on the direction of the angular momentum vector. Thus if one can assemble all the circles belonging to a common energy into a hyperspherical surface by lifting each one into a fourth dimension, one has something of Fock's momentum space representation.

Vectorial methods gradually came to replace the quaternionic analysis introduced by Hamilton, and set forth in great detail in the two editions of his treatise. Thus we find a solution of the Kepler problem in Gibb's and Wilson's book (5) on vector analysis in which the "Runge" vector plays a prominent role, and finally in the widely used monograph on vector analysis of Runge (6), which appears to be the source of the inspiration for its modern usage, even though as we have seen, this was by no means the earliest at which such a vector was known. Nevertheless its existence and convenience in the derivation of the equations of planetary motion were commonly enough known that Pauli (7) was able to make immediate use of it in 1926 in operator form, along with the operator corresponding to the angular momentum, to treat the hydrogen atom by means of Heisenberg's matrix mechanics. He drew in turn upon Lenz' (8) use of the Runge vector in 1924, in conjunction with the angular momentum vector, to describe the hydrogenic orbits according to the old quantum mechanics. Lenz had done so as a prelude to analyzing the perturbation in the motion and spectrum caused by superimposed uniform electric or magnetic fields. Indeed, if we are to believe historical testimony concerning that era (9), the elegance of Pauli's solution was a critical factor in securing the acceptance of matrix mechanics, with its operational methods.

Klein, no doubt remembering his earlier treatment of the spherical top, had been able to comment in 1933 that the components of the angular momentum and the Runge vector together satisfied the commutation rules for the generators of the four-dimensional rotation group, as Hulthén (10), reported in presenting a simplified version of Pauli's derivation. Podolsky and Pauling (11) had exhibited the momentum space wave functions in 1929, and in 1932 Hylleraas (12) had obtained the differential equation for the hydrogenic wave functions in

momentum space. So, it would seem that the knowledge of the necessary constants of the motion and their commutation rules was current in the time of Fock's paper. Nevertheless, the integral rather than the differential formulation of the momentum representation and the subsequent introduction of the stereographic projection in momentum space were the essential ingredients in giving a simple geometric interpretation of the true symmetry of the problem. Once this was done, Bargmann immediately made the connection to group theory by relating the symmetries to the transformations generated by the constants of the motion.

Since constants of the motion for the hydrogen atom and the formalities of their commutation rules were known when Fock's paper was written, it is evident that his lucid geometric interpretation of their corresponding symmetries was indispensable in promoting the concept of a "hidden" symmetry, if for no other reason than the fact that it was the lack of such a concrete picture which originally motivated the adjective "accidental" for the prevailing degeneracies. His technique of stereographic projection invited the scrutiny of other potentials to see whether other degeneracies could receive a similar explanation. In the meantime Laporte and Rainich (13) were investigating a problem in differential geometry which had arisen from a modified electrodynamics proposed by Born, which led to a slightly different concept of minimal hypersurface than the customary one. The study of such surfaces showed that they possessed a type of symmetry in a space of lower dimensionality which could be induced by spherical symmetry in a space of higher dimension if a stereographic projection were made between the two. Laporte (14) showed that these precepts led just precisely to the hydrogenic symmetry which Fock had discovered.

One conclusion to be drawn from the work of Bargmann and Fock was that if it was possible to find a collection of classical constants of the motion whose commutation rules with respect to the Poisson bracket yielded a recognizable Lie algebra, one might hope to find quantum mechanical operators whose commutator brackets might be used for the same purpose. Such a procedure would not be entirely unambiguous, since in the case of the hydrogen atom the commutation rules already depended upon the energy, and it was seen that manifolds of different energy could have different symmetry groups. In this case the Lorentz group, an Euclidean group, or the four-dimensional rotation group arose according to the value of the energy. However, if it should happen that the commutation rules involved some other quantity than the energy, it might be difficult to consider the commutation rules as defining a Lie algebra. Since the energy is a constant of the motion, too serious a problem does not arise when it appears in the commutation rules, since it can always be replaced by its value, classically, and its eigenvalues, quantum mechanically. Another, more serious, problem lies with the correspondence between a classical function of the coordinates and momenta and a quantum mechanical operator, since the quantum operators corresponding to coordinates and momenta do not commute. In the case of the Runge vector, it was possible to find a suitably symmetrized form of the operator by inspection, but one could hardly hope that more complicated constants would succumb to the same improvisation.

### III Symmetry of the Harmonic Oscillator

In spite of such misgivings, the next system to receive attention was the harmonic oscillator. The constants of the motion of an isotropic harmonic oscillator are algebraically far simpler than those of a hydrogen atom, but nevertheless it seems that only the existence of the angular



momentum had ever been suspected. Most likely the ease of solving the equations of motion of the harmonic oscillator, both classically and quantum mechanically, forestalled an active interest in finding the constants of the motion, whereas the Runge vector plays a very useful role in obtaining as well as exhibiting the solution of the hydrogenic problems. Nevertheless the awareness of the importance of knowing the symmetry group aroused by Fock's exposition of the symmetry of the hydrogen atom could hardly have failed to create interest in the symmetry of the harmonic oscillator, whose degeneracy was as well known as that of the hydrogen atom, and which is one of the most fundamental of all quantum mechanical systems.

The unitary unimodular group was found to be the symmetry group of the isotropic oscillator by Jauch (15) in 1939; a result which formed the principal content of his University of Minnesota doctoral dissertation (16), and which he and Hill published the following year in the *Physical Review* (17). A much more detailed treatment of the oscillator symmetry and related material including some historical and philosophical material on the development of quantum mechanics formed a very delightful set of seminar notes prepared by Hill (18), some years later, in 1954.

As had happened earlier with the hydrogen atom, the symmetry group of the oscillator was at first known only through the commutation rules of its constants of the motion. The geometric visualization which Fock's transformation had achieved was not immediately forthcoming, and in fact Jauch and Hill complained about the lack of apparent physical significance of some of their constants. The particular case of the two-dimensional harmonic oscillator was an interesting curiosity because it was definitely the unitary unimodular group and not its factor group, the three-dimensional orthogonal group, which was the symmetry group. This was a distinction which could readily be demonstrated because the two-dimensional oscillator has degenerate levels of every integer multiplicity, and only odd-dimensional representations can occur for the rotation group. Previously the group  $SU(2)$  had always been associated with relativistic effects and spinning electrons, and not with purely classical problems.

It remained for Saénz, a student of Laporte, in his 1949 dissertation (19), at the University of Michigan, to exhibit a geometrically significant canonical transformation, whereby the phase space of the harmonic oscillator could be regarded as a complex vector space and the constants of the motion interpreted as generating unitary unimodular transformations of the phase space. The technique was to use the stereographic parameters of Laporte and Rainich, which in fact are the action-angle variables for the harmonic oscillator when properly parameterized.

The appearance of the harmonic oscillator Hamiltonian as a sum of squares of coordinates and momenta makes it very tempting to write it in a complex form, to which unitary transformations may be applied; but care must be taken to ensure that the unitary transformations are canonical, to preserve the spirit of Hamiltonian mechanics. Such an explanation of the unitary unimodular symmetry of the harmonic oscillator was published by Baker in 1956 (20).

The constants of the motion of the harmonic oscillator can be combined in complex form in such a way as to obtain the product of a creation and an annihilation operator; this interpretation also has a high intuitive significance, and suggests that other symmetry groups might be interpreted in terms of ladder operators.

At first sight, the analysis which applies to the isotropic harmonic oscillator ought to apply to the anisotropic oscillator as well, especially if one bears in mind the interpretation in terms of ladder operators and the exchange of quanta of energy between different coordinates. Jauch and Hill had found classical constants of the motion of the anisotropic two-dimensional oscillator, when there was a rational frequency ratio between the coordinates, but they found

that the most reasonable quantum mechanical operator which they could construct based on the classical constants did not quite satisfy the proper commutation rules to define a Lie group. Dulock (21), in his University of Florida dissertation of 1964, managed to extend the classical constants to the general case of arbitrary frequency ratios, but it was even less clear how to form the quantum mechanical operators, in view of the transcendental nature of the constants.

Demkov (22), succeeded in avoiding the deficiencies in the commutation rules of the quantum mechanical ladder operators for the anisotropic oscillator — in particular for the case of a 2:1 frequency ratio — by dividing the states into two groups (of even and odd total energy, respectively) each one of which belonged to a unitary unimodular symmetry group. His student, Il'kaeva (23), treated a somewhat more general case, but as recently as 1968 Vendramin (24), published a claim that the unitary unimodular group cannot be the symmetry group of an anisotropic harmonic oscillator. Precisely stated, his claim is that the states of the anisotropic oscillator cannot belong to only one series of irreducible representations of the unitary unimodular group, which is in fact correct. Cisneros (25a) has unraveled the symmetry group of such systems, and has found that multiple families may occur, and additional degeneracies due to unitary groups of lower dimension when there are special relationships among the individual frequencies. That the representations of the unitary unimodular groups are reducible for rational frequency ratios was also analyzed by Maiella and Vilasi (25b).

Strictly speaking, the Jauch-Hill constants of the motion do not form a complete set of commuting constant for the anisotropic oscillator and one must additionally take into account some purely quantum mechanical operators. These operators determine the parity of the energy levels, or in the more general case, their residue classes with respect to the frequency of the individual oscillators. One has the interesting situation that the less commensurable the frequency ratios, the more families of representations of the unitary group occur, and the greater is the distance from the ground state to the first degenerate level. In the limiting case of incommensurability, the one-dimensional representation occurs infinitely often, and the gap to the first degenerate level is infinitely high, so to speak. In this way one can reconcile Dulock's result that even the incommensurable anisotropic oscillator has the symmetry group  $SU(n)$  with the evident lack of any degeneracy, which would be untypical of a symmetry group.

The theme of Saézn' dissertation, which was aimed at an understanding of the symmetry of Dirac's equation for the hydrogen atom, was to reduce those systems wherein accidental degeneracy was known to occur to force-free motion on the surface of a hypersphere. The spherical top is another system which may be treated in such terms, although in that case the term "accidental" degeneracy is inaccurate because the hypersphere is the natural configuration space for the problem. We have already remarked that the rigid rotor was generally classified along with the harmonic oscillator and the hydrogen atom as a system showing accidental degeneracy, and for this reason it is interesting to find that there is a uniform treatment of all three systems.

## IV Symmetry of Tops and Rotators

The whole subject of tops and rotators has had a long history and an extensive literature, especially in classical mechanics, and was highly developed long before the advent of wave

mechanics. Perhaps the most distinguished treatment of the theory of tops is the monumental four-volume work of Klein and Sommerfeld (26), published in 1897, wherein the motion of tops, gyroscopes, and rotating systems in general is given an exhaustive treatment. These objects also figured prominently in the old quantum mechanics, since they form the natural model for the treatment of the rotation of molecules, and were very promptly investigated when the new quantum mechanics began to make its appearance around 1926. The proper formulation of Schrödinger's equation for the rigid rotator required some thought, simply because three-dimensional space is not its configuration space. Rather, the "coordinates" are Euler's angles or some similar rotational parameters, and it was necessary to understand how to write a proper wave mechanical analogue of Euler's equations for the motion of a rotating body. On the other hand, it was possible to treat the rotator at once in the matrix mechanics, due to the ease with which the principal moments of inertia could be used as coefficients to write the Hamiltonian as a sum of squares of the angular momentum operators, and its eigenvalues obtained by operational methods.

In the years around 1920 the old quantum mechanics was used for the study of tops and rotators, notably by Epstein (27), Reiche (28), Kramers (29), and Kramers and Pauli (30), some of it based on an analysis of the equations of motion made years earlier by Kolossoff (31). Not surprisingly, they were among the first examples taken, both in the matrix mechanics and in the wave mechanics, but it was not long before explicit treatments appeared. Dennison (32), Reiche and Radamacher (33), Witmer (34), Kronig and Rabi (35), and Lütgemeier (36) made some of the earliest contributions. From the point of view of symmetry, and especially of the spherical top, Hund's (37) treatment of the spherical top in quaternionic coordinates, and Klein's (38) 1929 determination of the commutation rules so that he could analyze the asymmetric rotor by operational methods are the most relevant.

The asymmetrical top received its most extensive treatment in a series of papers by Kramers and Ittman (39), also in 1929, with some further contributions by Wang (40), and Ray (41). Casimir's thesis of 1931 (42) discusses the quantization in terms of generalized coordinates, and the commutation rules of the angular momentum operators. There the matter rested for two decades, until the availability of microwave equipment in the late 1940s permitted a thoroughgoing experimental analysis of molecular rotational spectra, and with it further studies of the quantum mechanics of rotating systems.

The principal new techniques to have emanated from this recent period are operational methods, not only for the determination of energy levels and wave functions, but for dipole and quadrupole transition matrix elements and other such information. Additionally, the advent of electronic computers has permitted the application of all these techniques to an array of configurations which would previously have been completely impossible. Some of this material is to be found in the series of papers initiated by King et al. (43), in the *Journal of Chemical Physics*, while the diverse operational techniques were published by Burkhard (44), and Shaffer (45).

In a sense, the degeneracy and symmetry which one encounters in the family of tops is not accidental, any misapprehension to the contrary having most likely arisen from the hasty assumption that three-dimensional space is their configuration space, and that the Hamiltonian, rather than the Eulerian equations, have been applied. In reality, the four-dimensional unit sphere is the most convenient parameter space for the treatment of rigid motion and, if anything, one should expect the four-dimensional rotation group to be the one governing symmetries. For a better understanding of this situation one ought to take note of

the different classes of “rotors” which the spectroscopist recognizes, as well as enumerating their characteristic degeneracies.

First of all, there is a difference between a “rotator” and a “rotor” or top. The former is merely a point rotating about some center, possessing an energy in virtue of its angular momentum. Its radial distance is constant; for example, if a massive point is connected to a fixed center by a light rigid rod. Its wave functions will be ordinary spherical harmonics, and its eigenvalues are those of the square of the angular momentum operator. It manifests a degeneracy in the  $z$  component of its angular momentum on account of the spherical symmetry of such a configuration.

Such an arrangement, however, is not what one would customarily regard as a “top” because it describes the motion of a point, perhaps even a rod, but not the rotational motion of a solid body. At best, it can be regarded as characteristic of a body one of whose moments of inertia is zero. Turning to true tops, if all three moments of inertia are equal and nonzero, the body is called a spherical top. Quantized, it shows a very high degeneracy, characteristic of the four-dimensional and not the three-dimensional rotation group. Such degeneracy is  $n^2$ -fold,  $n$  being a principal quantum number. Now, if only two moments of inertia are equal, but distinct from the third, the top is called a “symmetrical” top, and has a degeneracy  $2(2\ell + 1)$ , which is double that of a spherically symmetrical system, in spite of the fact that a body with such moments of inertia does not have spherical symmetry. Finally, when all three moments of inertia are different, the object is called an “asymmetrical top” and surprisingly enough it still shows a degeneracy in its energy levels  $(2\ell + 1)$ , characteristic of spherical symmetry.

What do we mean by the “configuration space” of a top? It is hardly three-dimensional space, which is suitable for describing the location of points comprising the top, but has to be formed from some sort of collective coordinates, such as their center of mass, or in the present case, parameters describing the orientation of the body in space. One very convenient set of parameters for this purpose are the Euler angles, which may be used to specify the orientation of a set of coordinates attached to the body, in terms of a fixed set of coordinates attached to the laboratory. Analogous parameters may describe rotations in a space of any number of dimensions, but in three dimensions, we first may rotate the  $z$  axis to a new position, which requires two coordinates — let us say the colatitude and azimuth of the new  $z$ -axis. This determines the orientation of the new  $x$ - $y$  plane, but not the location of the  $x$  axis within the new plane, so that a third angle must be specified. The result is three coordinates, the three Euler angles, which must range over a *three*-dimensional manifold, and not a two-dimensional manifold which ordinarily specifies angular orientation.

There are many ways of parameterizing an element of the three-dimensional rotation group, and for many purposes one of the most convenient is the use of unit quaternions, whose coefficients in such a representation are the Cayley-Klein parameters of the rotation. Since the unit quaternions range over the surface of the hypersphere, a three-dimensional manifold, it is in this way that the hypersphere becomes the natural configuration space of the top problems. The relationship is a very curious accident of three dimensions, for it is only in this one exceptional instance that the parameter space for a rotation group is a sphere. Of course, one will obtain wave equations for tops of other dimensions, with their appropriate degeneracies, but there would not result quite the elegant picture which one obtains in three dimensions, that the motion of the spherical top is equivalent to force-free motion on the surface of a hypersphere. Since the motion of the spherical top can be so characterized, there results the rather nice uniform interpretation of the accidental degeneracy of three of the most

important idealized systems in quantum mechanical theory, which was expounded by Saénz in the first half of his dissertation.

In explaining the accidental degeneracy of the hydrogen atom one has to introduce stereographic coordinates in momentum space, which allows the reduction of the motion to force-free motion on the surface of a hypersphere, for negative energies. For the harmonic oscillator, the action-angle variables for an uncommon, but not unreasonable, coordinate system again allow an interpretation of the motion as force-free motion on the surface of a hypersphere. For the spherical top, it may be demonstrated that the equations of motion are again those of force-free motion for a particle constrained to reside on the surface of the hypersphere. However, we have a rather more direct way in which to relate motion on the hypersphere to the actual movement of the top, which contrasts with the considerably more indirect interpretation which must be given to rotations of the hypersphere in the other two problems. Since rotation of a body is detected by noticing the difference in orientation between a system of coordinates fixed to the body and a set fixed in the laboratory, it seems that we may rotate either one or the other of these coordinate systems at will. Rotating the set attached to the laboratory results in a new motion derived from the old by a rotation, and hence is a symmetry of whatsoever top, spherical symmetrical or asymmetrical. Rotation of the set attached to the body is immaterial for the spherical top, is a symmetry if performed about the symmetry axis of the symmetric rotor, and results in no symmetry at all for the asymmetric top. The four-dimensional rotation group is a direct product of two three-dimensional rotation groups, and in the case of the motion of a top, the two constituent factors can be identified with the external rotations (of the laboratory coordinates) and the internal rotations (of the body-fixed axes). Rotation of the laboratory coordinates will always be a symmetry operation, but the internal rotation group will be restricted according to the number of principal moments of inertia which are equal. Thus the spherical top will have the full four-dimensional rotation group as a symmetry group, the symmetric top will have the direct product of the three-dimensional group with the rotations about the symmetry axis, and the asymmetric rotor will only have a reflection group for its internal symmetries.

## V Bertrand's Theorem

The state of affairs as Saénz presented it in 1949 was reasonably complete. The three most widely known systems in which accidental degeneracy above and beyond that required by spherical symmetry was known to exist were shown either by an appropriate choice of coordinates or an appropriate canonical transformation to be equivalent to force free motion of a particle confined to the surface of a hypersphere (or in the case of the positive or zero energy states of the hydrogen atom, a closely related surface). Some slight extensions of this result in other directions was known. For example, although a physicist would naturally give his predominant attention to three-dimensional systems such as occur in the real world, some two-dimensional systems were considered important enough to treat, and sometimes results were stated generally for an arbitrary number of dimensions. For example, Jauch and Hill had shown that a transformation similar to Fock's would account for the two-dimensional hydrogen atom, and Saénz' results were stated in quite general terms even if they were only applied to the familiar low-dimensional systems. In 1958 Alliluev (46) extended the stereographic technique explicitly to the hydrogen atom in spaces of an arbitrary dimensionality,

and Loudon (47), in 1959 found an unexpected degeneracy for the one-dimensional hydrogen atom, although this conclusion rests on some delicate assumptions concerning the appropriate boundary conditions for the Schrödinger equation which are not as yet understood to everyone's satisfaction.

Arguments existed to the effect that these were the only systems which ought to have exhibited accidental degeneracy, although there were sufficient loopholes in the argument to admit a number of other known highly degenerate systems. For example, the Kepler problem in non-Euclidean spaces was known to behave much like its Euclidean version, although the discrete spectrum was finite in a hyperbolic space (48), and the spectrum of the unbound states was discrete in spherical space (49). Even a free particle enclosed in an impenetrable cubic box also showed more degeneracy than cubic symmetry would require (50).

The usual argument supporting the uniqueness of the harmonic oscillator and Keplerian potentials in forming accidentally degenerate systems is an appeal to Bertrand's (51) theorem enunciated in 1873, which states that in problems where the kinetic energy is the sum of the squares of the velocities (which exempts non-Euclidean spaces and vector potentials) and the potential is spherically symmetrical (which exempts the cubical square well and anisotropic harmonic oscillator), the only potentials with bounded closed orbits are those for  $V(r) = -Ze/r$  (Coulomb potential) and  $V(r) = \frac{1}{2}kr^2$  (harmonic oscillator). As we have remarked, the degeneracy of the tops is not technically "accidental." The reason for the strict limitations in Bertrand's theorem are of course due to its method of proof, since one separates the Hamilton-Jacobi equation with the assumed potential and kinetic energies, assumes the existence of a circular orbit, and makes a perturbation calculation to see whether orbits near the circular one are also closed.

Bertrand's original paper is nowadays rather inaccessible, but fortunately there is an excellent exposition of the theorem and discussion of accidental degeneracy in a recent article of Greenberg (52). The same lines of reasoning could well enough be applied to systems with different forms of kinetic energy. Such an analysis was actually made by Darboux (53) for motion confined to a surface of revolution, a few years after Bertrand's theorem was published. He likewise investigated the possible force laws which could produce elliptic orbits (54a). An extension of Bertrand's theorem which is of interest for the movement associated with a magnetic monopole and some similar fields was published by Lehti (54b), in 1968.

Implicit in an application of Bertrand's theorem to limit the number of accidentally degenerate mechanical systems is the assumption that accidental degeneracy is to be equated with the existence of bounded, closed orbits; or in any event with orbits which are not space filling. There is also an implicit assumption that the existence of such orbits in the classical problem will be a reliable indicator of the degeneracy in the quantum mechanical problem.

Since the mathematical understanding of these conditions has never been completely decisive, there has grown up a considerable folklore about the nature of accidental degeneracy, reflecting to a considerable extent people's aesthetic feelings about how the resolution ought to appear. Mainly, we know of certain conditions under which accidental degeneracy will arise, but it is largely a matter of faith (and our limited range of experience) that there will be no accidental degeneracy when these conditions are absent. More bluntly put, we know some sufficient conditions for accidental degeneracy, but we do not as yet know any necessary conditions expressible in intuitive physical terms. One of the more attractive tenets of the folklore has been that accidental degeneracy arises from hidden symmetry, as has been amply demonstrated by the major examples. Hidden symmetry of course implies a symme-

try group, from which degeneracy follows in a pattern dependent upon the occurrence and dimensionalities of the irreducible representations of the group of the hidden symmetries.

Assume, as most often seems to be the case, that the symmetry group is a continuous Lie group. It will have a certain number of infinitesimal generators, which will necessarily be constants of the motion. Quantum mechanically, these generators will transform eigenfunctions of the Hamiltonian into other eigenfunctions, and so the possibility for degeneracy exists, unless the Hamiltonian and the constants of the motion have exactly the same eigenvectors. This is not possible when there are several noncommuting constants of the motion, say when the symmetry group itself is non-Abelian. Classically, the constants of the motion must generate transformations of orbits in manifolds of constant energy so that the more independent constants which exist, the more automorphisms of the constant energy manifolds we will have to work with.

For the case of a symmetry group, these remarks are but an informal statement of Schur's lemmas and the mechanism by which symmetry results in degeneracy. However, the existence of an adequate number of independent constants of the motion from whatever source they may arise will also produce degeneracy. One such source might be the separation of Schrödinger's equation (or alternatively the Hamilton-Jacobi equation) in several distinct coordinate systems. Separability in several coordinate systems is known to be related to the existence of orbits that are not space filling, as well as to classical degeneracy.

The reasoning is the following: If the Hamilton-Jacobi equation is separated, and action-angle variables exist, the existence of distinct frequencies for the angle variables will result in a Lissajous figure type of motion which will fill a region of phase space if the frequencies are incommensurable. The boundaries of the region will be surfaces where one or another coordinate takes an extreme value, so that the coordinate surfaces will be inherently defined by the orbits. For the bounding surfaces to coincide for two distinct systems of coordinates, the frequencies must be commensurable if not actually equal, which is just the meaning of classical degeneracy. Since separability of the Schrödinger equation goes hand in hand with separability of the Hamilton-Jacobi equation the reasoning may be extended from the classical to the quantum mechanical version of a problem. We may therefore always suspect a classically degenerate problem of originating a quantum mechanically degenerate version.

Degeneracy in a classical problem may also tell us something about its constants of the motion, as to whether they are algebraic functions of the coordinates and momenta or not. For, if a problem has a complete set of algebraic constants, one may define the coordinates and momenta in terms of them. For the moment we would want to define one coordinate in terms of another and some of these algebraic constraintss, which would imply that one coordinate was a finite-valued function of other, and hence the orbit could not be space filling. We can therefore infer that when a system has a complete set of algebraic constants of the motion, it would be classically and thereby quantum mechanically degenerate. Few systems satisfy this requirement; an important theorem demonstrated by Poincare at the beginning of the century denied such a possibility for the three-body problem in celestial mechanics, for example.

Summarizing the foregoing analysis, we can reach several tentative conclusions.

1. Symmetry, hidden or open, produces a degeneracy, to a degree depending on the noncommutability of the generators of the symmetry group.
2. Constants of the motion do the same. Since the Poisson bracket (or commutator) of two constants will be another constant of the motion, they will generate a Lie group whenever

the set is so closed, but they will induce degeneracy regardless.

3. For a system to be separable in more than one coordinate system, orbits must not be space-filling. In this case there will be an abundance of separation constants.

4. When there is a complete set of algebraic constants, the orbits will not be space filling. Not many problems are known with such a set, and some are known not to be so endowed.

5. When the kinetic energy has its usual form and the potential is spherically symmetric, the only potentials for which no orbit is space filling are the Kepler and harmonic oscillator potentials. These, by explicit construction, are known to have, respectively,  $O(4)$  and  $SU(3)$  as symmetry group accounting for their accidental degeneracy.

Basing one's conclusions on the above analysis, it is seen that Bertrand's theorem does not state that the known degenerate systems are the only ones, but it does ensure that other systems will either have space filling orbits or violate such assumptions as spherical symmetry of the potential or the Euclidean form of the kinetic energy. Since problems with space-filling orbits are not classically degenerate, it seems somewhat unlikely that they would be found to be quantum mechanically degenerate.

One precaution which must be observed in reviewing these conclusions is that the considerations have not always been stated with full mathematical precision and the results deduced and stated rigorously. This will be seen to lead to some further loopholes. Nevertheless, we have a fair representation of the situation as it existed until very recently, and as expounded in several sources Saénz (19), Greenberg (52), or Whittaker (55), for example.

## VI Non-Bertrandian Systems

Up until about 1963 the theory of accidental degeneracy was rather much as we have outlined it. Of all the textbook systems which were commonly studied, the spherical top, isotropic harmonic oscillator, and hydrogen atom showed far more degeneracy in their spectra than as required by their readily perceived spherical symmetry. However, it was possible to show that there was in reality additional symmetry present, adequate in each case to account for the observed degeneracy. For the spherical top, it was primarily a matter of understanding clearly that the coordinates were the angular orientation of the top and not the three Cartesian coordinates, and thus not an accidental degeneracy after all. Since the isotropic harmonic oscillator has constant energy surfaces which are spheres in six-dimensional phase space, it is perhaps not surprising that it has a symmetry group consisting of a subgroup of the six-dimensional rotation group which preserves the canonical structure of phase space, which we have seen turns out to be isomorphic to the unitary unimodular group  $SU(3)$ . Finally, Fock's stereographic mapping interpreted the  $O(4)$  symmetry group of the hydrogen atom as another symmetry inherent in phase space, which did not arise from purely geometric transformations in the configuration space. At the same time there were variants on these basic systems of different dimensionality, the anisotropic harmonic oscillator, tops with unequal principal moments of inertia, which could be understood in the same general terms, even if, as in some cases of the anisotropic harmonic oscillator, many ramifications of their symmetry remained obscure.

Additionally, arguments such as the ones we have just cited regarding Bertrand's theorem existed which tended to show that there might not be too many other accidentally degenerate



systems, but because they were not stated with mathematical precision, and because there were so many counterexamples when even the most obvious restrictions were violated, the subject could never be quite considered as closed. Among the counterexamples were the problems of motion in non-Euclidean space or in the presence of magnetic fields, which one felt would be similarly restricted when the theory was broadened to include more general types of kinetic energies. Likewise, the requirement of spherical symmetry excluded from the purview of the theory such interesting systems as the anisotropic oscillator, and theoretically important systems such as the cubic square well.

Beyond such tangible uncertainties, one could never be sure that even in those systems for which the degeneracy was supposedly resolved, the day would never come when an even bigger group would be discovered, producing the same pattern of accidental degeneracies, but encompassing constants of the motion which could be important in some as yet unforeseen context. One felt that accidental degeneracy was sufficiently accounted for when he found a hidden symmetry group such that each of its irreducible representations occurred no more than once in the system under consideration, although not all of them need necessarily occur. For example, only the symmetric tensor representations of  $SU(3)$  occur in the harmonic oscillator Hamiltonian, and only the representations of dimension  $n^2$  of  $O(4)$  occur among the hydrogen atom bound states,

When a given representation occurs no more than once in the wave functions of a given Hamiltonian, the mere knowledge of the symmetry group is sufficient to diagonalize completely the Hamiltonian; in fact this is the criterion by which one usually accepts the contention that the hidden symmetry is extensive enough to account for all the degeneracy present. Yet there is no hard and fast rule to judge at what point one has found an adequate amount of symmetry, since it is not feasible to work with the group of “all operators which commute with the Hamiltonian.” The extent to which matters have still been left to our judgement has been emphasized by Demkov (22).

We might also remark that such a criterion might be considered too severe. For instance one might find the energy levels of a Morse potential, or even of a mildly perturbed hydrogen atom, and find that the three-dimensional rotation group accounted perfectly for all the degeneracy present, namely the degeneracy in the  $z$  component of the angular momentum. Nevertheless, any given representation of the rotation group will occur infinitely often, so that finding wave functions having the symmetry of the symmetry group will by no means determine the eigenfunctions, even though it may simplify the secular equation for the entire system considerably. In this sense we receive considerably more than we bargain for when we determine the hidden symmetry group of the harmonic oscillator or the hydrogen atom.

As a final commentary on the folkloric aspects of accidental degeneracy, we ought to notice that in the harmonic oscillator and the hydrogen atom, the two foremost examples of accidental degeneracy which we have, the constants of the motion are, respectively, a tensor and a pair of vectors. Moreover, the trajectories in the two problems, both ellipses in the bound states, have, respectively, two perihelia and aphelia for the harmonic oscillator, and a single pair for the hydrogen atom. In fact, the existence of an integral number of such maxima and minima in the radial distance plays an important role in the proof of Bertrand’s theorem. These observations have sometimes brought forth the wistful thought that there might be a whole hierarchy of tensors, spinors, and such things, each with “its” own characteristic potential and whose components might be the generators of a hidden symmetry group for that potential. Thus far this family has never grown beyond its original two members, even

though this viewpoint has led to some interesting results concerning the type of potentials which might experience such constants of the motion.

We have been discussing almost exclusively nonrelativistic systems described by Schrödinger's equation. This does not imply that there was no interest in relativistic systems, although there is a far lesser incidence of degeneracy in the physically interesting instances of Dirac's equation. First of all, the relativistic harmonic oscillator does not make much sense on account of its ever-increasing potential, so that only the relativistic hydrogen atom remains, amongst potentials of general interest. But, the relativistic mass change spoils the simple closed elliptic orbits of the nonrelativistic theory, and with them the degeneracy in the principal quantum number of the Dirac equation's eigenvalues. A twofold degeneracy remains, due more to spin effects than to the Coulomb potential, beyond the azimuthal degeneracy to be expected from the spherical symmetry of the Coulomb potential.

Whatever the state of accidental degeneracy, or its theoretical or aesthetic importance, it found an important application around 1958 in the work of Elliott (56) and since that time has permeated the literature of nuclear physics. Of the constants of the motion of the harmonic oscillator, which generated the unitary unimodular group of symmetries  $SU(3)$ , there were two types which had a long-standing physical significance. Namely, these were the components of angular momentum  $L_{ij} = q_i p_j - q_j p_i$  and the energy differences between pairs of coordinates,  $D_{ij} = \frac{1}{2}(p_i^2 + q_i^2) - \frac{1}{2}(p_j^2 + q_j^2)$ . The remaining constants of the motion,  $K_{ij} = q_i q_j + p_i p_j$ , to a certain extent measure the "correlation" between the motion in the  $i$ th and  $j$ th coordinates, and one may attribute their existence to the fact that the frequency of a harmonic oscillator is independent of its amplitude. Thus, for example, if several particles moving independently in a harmonic oscillator potential are all clustered at the origin in a certain moment, they will all return again to the origin simultaneously, and thus they will seem to exhibit "collective" motion, even though they are in reality uncoupled. For this reason the assumption of a harmonic oscillator potential, at least as an approximation to a certain part of the nuclear potential, has found a certain popularity in nuclear physics. Moreover, the fact that the quadrupole interaction has a simple expression in terms of harmonic oscillator constants of the motion has made it a relatively tractable problem to form the proper linear combinations of degenerate harmonic oscillator wave functions, to diagonalize the quadrupole interaction, and to proceed from there with a discussion of nuclear shell theory.

The quantity of literature presently devoted to the nuclear shell model, and its treatment in terms of  $SU(3)$  and a wide variety of other Lie groups, makes it impractical for us to make any bibliographical citations, but as a final remark we might note that Moshinsky (57), in 1962, proposed that similar techniques might be found useful in molecular problems, exploiting the  $O(4)$  degeneracy of the Coulomb potential. More recently, he has applied the  $SU(3)$  techniques directly to such problems.

Another train of thought which started at about the same time as Elliott's was also motivated by the observation of certain regularities in the spacings of nuclear energy levels, and their close similarity to the rotational bands which could be noticed in the spectra of tops of one kind or another. Here the interest was not quite so much in the determination of degeneracies, which had been the traditional role of group theory, but in the actual shape of the spectrum itself. While it was a novel idea to think of Hamiltonians in such terms, the existence of ladder operators for the  $z$  component of angular momentum was an example of the way in which a commutation relation between two operators could influence the form of their spectra. Goshen and Lipkin (58) found such pairs of operators among the constants of

the motion of the harmonic oscillator, and showed that Hamiltonians which showed rotational bands could be formed by using such constants.

The discovery of a practical application for the theory of accidental degeneracy and the emergence of the idea that operators might determine the shape as well as the degeneracy of the spectrum of a Hamiltonian naturally aroused interest in obtaining a more extensive understanding of accidental degeneracy, especially with the broader view of subsuming the entire spectrum within one irreducible representation of a sufficiently large group. Such a large group would not necessarily be a symmetry group, for as Goshen and Lipkin had shown, considerable information could also be gleaned from operators which did not necessarily commute with the Hamiltonian, provided that the two operators obeyed some other suitable algebraic relationship.

Before we analyze accidental degeneracy more critically, and outline the most recent developments, it is worthwhile to investigate some further problems which have been important in one respect or another, even though the central issue has been neither symmetry nor degeneracy. Such has often been the case when one dealt with unbounded systems, for had there been a symmetry group its irreducible unitary representations would generally have been infinite dimensional, so that such subtleties as the dimensionalities of representations would have gone unnoticed. To start with, since they are exempt from Bertrand's theorem, problems involving the motion of a charged particle in a magnetic field may exhibit a considerable symmetry and accidental degeneracy.

## VII Cyclotron Motion

One such example is the problem of cyclotron motion — the motion of a charged particle in a constant magnetic field. A readily solved problem in both its relativistic and nonrelativistic forms, it made its appearance in the earliest literature of wave mechanics: in papers by Darwin (59), and Kennard (60) in 1927. Later on, around 1930, there was a period of rather intense interest in the quantum mechanical behavior of magnetically deflected electrons which can be attributed to the fact that in those days there were well defined discrepancies in the experimental values of  $e/m$ , the charge-to-mass ratio of the electron, and even for  $e$  itself, as deduced from diverse experiments.

The classical treatment of the cyclotron problem (which was hardly yet known by that name) yielded a circular orbit whose radius was inversely proportional to the magnetic field strength, but Page (61), in 1930 had considered the possibility that the radius of curvature of the trajectory of the quantum mechanical wave packet might be different from the classical radius, and that the discrepancy might influence the value of  $e/m$  in the right direction. Unfortunately his solutions tended to bear out this point of view, but were quickly challenged by various authors, and a certain exchange of opinions followed. Uhlenbeck and Young (62) disputed the result; Landau (63) had considered the problem in his theory of diamagnetism in metals; Alexandrow (64) had given a solution; and it was also considered from the relativistic point of view by Plesset (65) and by Huff (66), who in 1931 finally pinpointed Page's error as having overlooked some of the possible solutions whose absence from the wave packet would bias its average radius of curvature. Whereas a definite solution was obtained for this nonrelativistic problem, the actual solution of the radial part of Dirac's relativistic equation for cyclotron motion seems to have been gotten by approximate methods; In 1932, Laporte

(67) discussed an application of the WKB method to obtain such a solution. Even in the present day there remains some discussion (68). Rabi (69) gave one of the first solutions for the Dirac equation with a uniform magnetic field.

After a lapse of some 20 years, the problem was again revived in a series of papers by Johnson and Lippman using the elegant operator techniques much exploited by Schwinger. They considered both nonrelativistic motion (70), in 1949, and relativistic motion (71), in 1950. They were explicitly concerned with constants of the motion, although they still did not mention the possible symmetries. Among their results were a pair of constants of the motion which located the center of the cyclotron orbit, but which obeyed the commutation rules of a pair of conjugate ladder operators. Thus, both coordinates of the center could not be simultaneously observed. The energy levels were infinitely degenerate, corresponding to the freedom to locate the center of the orbit anywhere in the plane perpendicular to the magnetic field.

The Hamiltonian for the cyclotron problem is

$$\frac{1}{2}(p - A)^2,$$

wherein one may conveniently choose the “symmetric” gauge

$$A = \frac{1}{2}B(-y, x, 0).$$

One thereby obtains a bilinear function of the canonical coordinates and momenta, which can be simplified considerably by transforming to a rotating coordinate system. This is the treatment generally used in engineering discussions of the magnetron, and allied literature. Unfortunately the latter articles rarely use even the vector potential, and are in no way concerned with symmetry or degeneracy problems. Nevertheless, the constants of the motion which are found in the rotating coordinate system carry over to the stationary system, and it is quite advantageous to be able to use the Hamiltonian of the rotating system. In any event, when one deals with a bilinear Hamiltonian, the Hamiltonian equations of motion become linear equations with constant coefficients, to which special methods may be applied. These aspects were discussed by Dulock and McIntosh (72) in 1966 when they superimposed a harmonic oscillator potential in order to remove the degeneracy arising from the arbitrariness of the positioning of the origin, and emphasize the resulting symmetry. Pure cyclotron motion as well as pure harmonic oscillator motion were obtained as limiting cases.

The possibility of perturbing the harmonic oscillator with a uniform magnetic field was noticed as long ago as 1928 (73). The combination is mathematically equivalent to an anisotropic harmonic oscillator, for which one expects to obtain bounded closed orbits only for certain combinations of magnetic field strength and harmonic oscillator force constant. Those would be the combinations which result in rational frequency ratios of the oscillator. In the limit of pure cyclotron motion one finds that the unitary unimodular Lie group appropriate to the harmonic oscillator contracts to von Neumann’s algebra of ladder operators; and in addition to the *quadratic* constants of the motion typical of the harmonic oscillator one finds that there are even constants of the motion which are *linear* in the coordinates and momenta.

Although the problem of cyclotron motion is really a rather simple one, particularly the nonrelativistic version serves to illustrate principles which are considerably obscured in more complex systems. First of all, a uniform magnetic field has an apparent translational symmetry

which is not shared by its vector potential, in whatever gauge. This means that the Hamiltonian is not translationally invariant, even though it yields equations of motion with such an invariance. Of course, the change of gauge arising from translation must be incorporated in the constants of the motion generating infinitesimal translations, with the result that Johnson and Lippman's constants are not simply the momenta, but depend on the coordinates as well. This same phenomenon appears in crystal lattices which are subjected to a magnetic field, and requires the use of magnetic space groups to properly accommodate the phase change in the wave function arising from the gauge transformation. As one sees in dealing with the symmetry of a magnetic monopole, rotational symmetries in the presence of a magnetic field are also modified by an infinitesimal gauge transformation, but such problems can be avoided with the cylindrically symmetric uniform magnetic field of the cyclotron motion.

An additional possible source of complications fortunately does not arise in the cyclotron problem; it is convenient to transform the equations to a rotating coordinate system to simplify the Hamiltonian equations and obtain their solutions. Had constants of the motion somehow arisen, which were explicitly time dependent in the original coordinates, one would only have obtained constant rates and not constants of the motion in the original coordinate system. Relativistic cyclotron motion has been particularly useful for the insight which it affords to the symmetries of the Dirac equation.

## VIII The Magnetic Monopole

Another magnetic problem which has attracted a surprising amount of interest is the problem of the motion of a charged particle in the field of an isolated magnetic monopole, first analyzed by Poincaré (74) in 1896. Since we no longer deal with central forces, the angular momentum is no longer conserved, and the motion is no longer necessarily planar. However, it may be thought that a certain amount of angular momentum resides in the magnetic field, and that a total angular momentum  $\mathbf{D}$  exists

$$\mathbf{D} = \mathbf{L} - \epsilon \hat{\mathbf{r}}$$

in which  $\mathbf{L}$  is the mechanical angular momentum  $\mathbf{r} \times \mathbf{p}$ , and  $\epsilon$  is the magnetic pole strength. The total angular momentum, already observed by Poincaré, is a conserved constant, and plays the role of the angular momentum when the magnetic pole strength is nonzero. In particular, where  $\hat{\mathbf{r}}$  is a unit vector in the radial direction, we have

$$\hat{\mathbf{r}} \cdot \mathbf{D} = -\epsilon$$

so that the motion of a particle in the field of a magnetic monopole is always confined to the surface of a cone whose half-angle decreases with pole strength from a value of  $\pi/2$  in the absence of a magnetic field. For the motion of a charged particle in the field of an uncharged monopole, the trajectory is a geodesic on the surface of the cone. The particle spirals in from infinity, is reflected, and recedes to infinity on a path asymptotic to an element of the cone.

Vectorial methods are quite adequate for treating the motion of a particle in a monopole field, and several articles using them may be found in the recent literature: Lapidus and Pietenpol (75), Nadeau (76), Lehnert (77). Quantum mechanical interest in the monopole dates from Dirac's (78) speculations of 1931 and Tamm's (79) solution of its Schrödinger

equation. One of their immediate conclusions was that if the monopole were to exist as an isolated particle, its magnetic charge would have to be quantized, and as an indirect conclusion one could deduce the necessity of quantizing electric charge as well. The next two decades saw attention being paid to various details: Grönblom (80) and Jordan (81) examined how critical the location of the singularity in the vector potential might be for the solutions, Saha (82) speculated whether a magnetic charge might account for the proton's greater mass than the electron, while Wilson (83), Eldridge (84), Saha (85), and Ramsey (86) made miscellaneous contributions or suggestions. Of more importance were Fierz' (87) alternative derivation of Dirac's and Tamm's results, where in particular the role of Poincaré's vector  $\mathbf{D}$  as the generator of infinitesimal rotations and the angular momentum of the field were given explicit treatment, and Banderet's (88) treatment of scattering from a monopole. Ford and Wheeler (89) made a semiclassical analysis of scattering from a monopole; Goto (90) speculated on their behavior in cosmic space, and Wentzl (91) wrote a short note on their properties. Harish-Chandra (92), solving the problem relativistically with Dirac's equation, found that not even the dipole magnetic moment of the electron would lead to a bound state with the monopole, a result which did not modify earlier conclusions about a non-spinning electron obtained from the solutions of Schrödinger's equation. The properties of an electrically charged magnetic monopole were investigated by Eliezer and Roy (93) using Schrödinger's equation, while Malkus (94) investigated the energy levels of a charged monopole using Pauli's approximation. Unfortunately the more exact treatment with the Dirac equation leads to a singular potential in the lowest angular momentum states (95).

With the exception of the last three papers in which an explicit electric attraction was included, no bound states were ever found, and so again questions of symmetry were relatively unimportant. Moreover, the magnetic field removes the accidental degeneracy of the Coulomb problem, so that the various authors would have had no reason to have been concerned with symmetries or degeneracy anomalies either. Since angular momentum is no longer conserved, rotational symmetry must be given a cautious treatment, but it would seem that only Fierz gave the matter much attention.

There is an appreciable number of experimental papers, concerned with continuing efforts to detect isolated monopoles, which to date have been uniformly negative. Additionally during the past decade there have been a number of papers treating monopoles from the point of view of quantum field theory. They have two motives: one to obtain additional information which might assist the efforts toward experimental detection, and the other to determine whether there would be any inconsistency or contradiction in field theory itself which might rule out the existence of monopoles. Some of the papers are noteworthy from the point of view of symmetry and degeneracy, particularly Schwinger's (96) arguments that the quantized pole strength ought to be twice that originally required by Dirac, and Peres (97) confirmation of this result from symmetry principles, which depend somewhat upon assumptions regarding the properties of angular momentum. Another potentially interesting paper (98) treats the angular momentum of the field from such an extrinsic point of view that it is hard to reconcile with the known symmetry properties.

In point of fact, symmetry in the presence of a magnetic field requires rather careful attention. Even though the magnetic field may possess a certain symmetry, such as translational invariance or spherical symmetry, the vector potential from which it is derived will more than likely not possess the same symmetry. A symmetry operation will therefore result in a gauge transformation. Since, in Hamiltonian mechanics, the vector potential is to be added to the

canonical momentum, any change in the vector potential produced by a symmetry operation will be manifested as a gauge, which will have to be canceled in the canonical transformation which is applied to the momentum operator. Therefore the generators of an infinitesimal symmetry transformation which one would expect in the absence of a magnetic field have to be modified by the infinitesimal gauge transformation which that symmetry operation produces. In just this way Poincaré's vector  $\mathbf{D}$  replaces the angular momentum for the spherically symmetrical monopole field, and in fact similar considerations can be seen to apply to the problem of cyclotron motion.

For the uncharged monopole, there is perhaps very little more to be said. For a charged monopole, the accidental degeneracy of the Coulomb field is lost, but it may be recovered in a way whose mathematical elegance outweighs its physical artificiality. This way is to add a repulsive centrifugal potential proportional to the square of the magnetic pole strength, whereupon both the Coulomb problem and the harmonic oscillator exhibit accidental degeneracy. The mechanism may be understood if we recall that the effect of a centrifugal potential is to cause an orbital precession. In the case of a central force the precession occurs in the plane of motion, and in the present case it takes place about the vector of total angular momentum. The most noticeable difference between central force motion with and without the magnetic field of the monopole is its confinement to the surface of Poincaré's cone, so that motion which would ordinarily be planar is simply rolled up on the surface of the cone. However, an orbit which would be closed in the plane will extend around more than one circumference on the cone. This effect can be counteracted by an appropriate precession.

The attempted recovery of our two classically degenerate systems in this manner leaves the harmonic oscillator still somewhat intractable, but the Coulomb potential acquires some quite surprising attributes. First of all, it is possible to construct a Runge vector based on the total angular momentum rather than on the mechanical angular momentum. It is no longer orthogonal to the angular momentum, either mechanical or total. It may be shown that the orbit is again planar, although our considerations only led us to expect that it would be closed. The monopole no longer occupies the focus of the conic section comprising the orbit, nor does it even lie in the plane of the orbit. Nevertheless, the Runge vector and the total angular momentum still generate an  $O(4)$  group of constants of the motion, classically as well as quantum mechanically, a group which is adequate to account for the degeneracy which is observed. Here there is something of a surprise, for the minimum angular momentum value which may occur is that determined by the quantized magnetic pole strength. Moreover, the irreducible representations which occur are not those of dimension  $n^2$  characteristic of orbital angular momentum, but rather those of dimension  $mn$ , where  $m - n = 2\epsilon$ . If one wishes to avoid wave functions transforming according to half-integral representations of the rotation group, and therefore which would be double valued, he is forced to accept Schwinger's value for the minimum quantized pole strength, rather than half that amount, which was Dirac's original quantum. This result depends to a considerable extent on the choice of gauge. Finally, even though the symmetry group is  $O(4)$ , some such transformation as Fock's to force-free motion on a hypersphere is ruled out, since the  $mn$  representations do not exist for orbital angular momentum.

As the folklore requires, our charged monopole is separable in a variety of coordinate systems, including polar, parabolic, quaternionic, and ellipsoidal. This latter system is interesting, inasmuch as it also allows the separation of the equation for a pair of charged monopoles with the repulsive centrifugal potential. A detailed treatment of the symmetry of

the monopole problems was given by McIntosh and Cisneros (99a). Two papers by Zwanziger (99b) also contain a wealth of detail, particularly regarding magnetic sources in the Maxwell equations, scattering from the monopole, and separation of the relative coordinates for the two-body problem.

Although the problem of classical motion in the field of a magnetic dipole is of considerable practical and theoretical interest, it is a vastly more complicated system to treat, starting with the nonseparability of the radial and colatitudinal coordinates in its Hamilton-Jacobi equation. Extensive work on classical motion in the field of a magnetic dipole, also including an attractive Coulomb potential, has been carried out by Störmer (100). The motion of cosmic rays in the magnetic field of the earth is thought to follow such a model, at least as an approximation. Quantum mechanically, such a system is of interest for its application to the scattering of neutrons, whose principal mode of interaction is through their magnetic dipole moment.

## IX Two Coulomb Centers

As we have seen, there is considerable opportunity for the occurrence of accidental degeneracy and hidden symmetry in problems involving motion in non-Euclidean spaces, and velocity-dependent forces. Since the considerations of Bertrand's theorem rule out power law forces other than those of the harmonic oscillator and Coulomb forces, one has to search among the noncentral forces to find further instances of accidental degeneracy. We have already remarked that the presence of magnetic forces, such as in the presence of a monopole or in a constant magnetic field, can originate degeneracies in some instances. However, in treating purely electrostatic forces, one of the first of these which comes to mind is the problem of motion under the influence of two charged particles, the two-center problem. It is a system which admits separation in prolate ellipsoidal coordinates, but which is not classically degenerate. The form of the solution does not change greatly if the force centers bear magnetic as well as electric charge, provided, as in the case of the magnetic monopole, that the repulsive centrifugal potential proportional to the square of the magnetic charge is also included. In ellipsoidal coordinates, the classical turning points are defined by fourth-degree polynomials so that elliptic functions are required to integrate the equations of motion. The orbit will be in general one which fills the volume of the figure of revolution bounded by two ellipsoids and by two hyperboloids.

With such classical antecedents one would not hold much hope for finding quantum mechanical degeneracy beyond that required by the cylindrical symmetry arising from rotating the system about the line joining the two centers, and in the case of equal charge on the two nuclei, reflection in the plane bisecting this line. Nor do the solutions of Schrödinger's equation which are available indicate accidental degeneracy, with the exception that at certain internuclear distances and with certain charges, crossings of energy levels do occur. Such crossings were supposedly forbidden by a theorem of von Neumann and Wigner (101), but it has been known, and recently been shown once again (102) that the existence of the separation constant (103) in spheroidal coordinates produces the vanishing term needed in the Wigner-von Neumann theorem. Alliluev and Matveenko (104) have tried to explain the crossing on the basis of accidental degeneracy, but unfortunately the situation still exhibits a number of complexities.

Part of the reason for this lies, of course, in the fact that the two-center problem is math-



ematically much more complicated than the simple one-center systems. Classically one finds that he does not obtain a chain of separated equations from the Hamilton-Jacobi equation, as he does for example in the hydrogen atom. In the hydrogen atom the  $\varphi$  equation unambiguously determines one constant, the  $z$  component of angular momentum, which may be substituted into the theta equation. This equation in turn determines the total angular momentum, which may finally be substituted into the radial equation to extract the energy as the final constant of the motion. However, in the two-center problem although the  $z$  component of the angular momentum is readily enough separated, the energy  $E$  and the separation constant  $\alpha$  appear in both the  $\xi$  and the  $\eta$  equations ( $\xi$  and  $\eta$  are the ellipsoidal coordinates). This mixture persists quantum mechanically, so that one obtains two differential equations, each involving two eigenvalues; a much nastier situation than the customary one in which each eigenvalue equation involves only one eigenvalue.

These complications are further compounded by the fact that the  $\xi$ ,  $\eta$ , and  $\varphi$  action integrals are related to the separation constants through complete elliptic integrals so that with the exception of some very special cases, such as one of the charges vanishing, their use as canonical coordinates will involve transcendental functions. Finally one has to contend with the fact that the classical solutions are also expressed in terms of elliptic functions, which makes the formation and discussion of ladder operators that much more complicated.

Historically the first attempt to quantize the two-center problem seems to have been made by Pauli (105), in 1922, using the old quantum mechanics, and it was not entirely successful — a failure which hastened the decline of the old quantum mechanics. The reason for this probably lies in the very nature of the two-center problem. Classically a tightly bound electron will circulate near one center or the other, but in quantum mechanics that is another matter. If the centers are near together, even though a wave packet is initially constructed with the particle's wave function concentrated at one center, it will eventually and perhaps rather rapidly diffuse into the neighborhood of the other. The eigenfunctions will have nonzero amplitude near both centers, and thus the electronic behavior is classically rather different from the quantum mechanical version.

In any event, wave mechanical calculations have been undertaken since the advent of the new quantum mechanics, and have continued until the present time. They may be grouped into three broad categories: direct attempts to integrate the Schrödinger equation, molecular orbital calculations, and semiclassical computations which are surprisingly simple and accurate.

There are two limiting cases with which comparisons can readily be made: the “united atom” in which the centers are very close in comparison to the potentials involved, and the “separated atom” in which they are very distant. In the former case, one has small perturbation of a dipole or quadrupole type of an atom with the total charge of the two nuclei, and thus very nearly a single hydrogen atom. In the other limit the system behaves as though it were composed of two atoms which influence each other through a weak Stark effect.

One may hope to interpolate between these two limits, and compare the levels with one symmetry at one limit with similar levels at the other limit. It is at this point that the “no crossing” theorem of Wigner and von Neumann enters. The only difficulty is that crossing, in fact, occurs, and thus there can be accidental degeneracy of certain levels at certain internuclear distances. The possibility for a more exact investigation of the entire degeneracy situation of the two-center problem still remains open.

In fact, one might remark somewhat on the philosophy of the two-center problem as it most often occurs in the literature. The interest has been not so much to find the complete set of energy levels for a nuclear pair at a fixed internuclear distance as it has been to find the energy of the ground state as a function of the nuclear separation. In this way one may hope to determine the binding energy of a diatomic molecule, at least one of such simple structure, and related information.

A limiting case of the two-center problem is the electric dipole, which has received attention in recent times due to the curiosity which exists as to whether or not it has any bound states. Here the problem is complicated by the fact that the potential of the dipole is a singular potential, meaning that it is of the form  $r^{-k}$ , for  $k \geq 2$ . This radial term is also modified by an angular factor in the dipole problem. Classically, the singular potentials possess divergent radial action integrals, so that a complete set of action-angle variables cannot be found! The precise case of  $k = 2$  has the unusual feature that there is a continuum of eigenvalues, even for the bound states. Case (106) has shown how one can still quantize such singular potentials, but additional information beyond the Hamiltonian — such as a specification of phase at the origin — is required. Classically the situation is rather similar, as it would not seem that Newton's equations alone are adequate to account for the particle's passage through the origin.

Singular potentials, and particularly the centrifugal potential, make an appearance in several situations. The classical motion under the centrifugal potential is a spiral, whose extent depends upon the energy of the particle. If the particle is unbound, it will spiral away to infinity, while if it is bound, it will spiral in to the origin and out again, but it spirals in at a constant angle to the radius vector and its precise position of emergence cannot be foreseen from Newton's laws. Some orbits are circular, but these are unstable against the slightest perturbation. An interesting feature of the Hamiltonian is its invariance under dilations. Any orbit may be dilated to obtain another orbit, although the time scale must simultaneously undergo a reciprocal adjustment.

This dilational symmetry manifests itself in the Schrödinger equation, in that a wave function may be dilated by any amount to obtain another wave function. Thus even though the wave functions are normalizable, one does not obtain a quantization of energy unless some supplementary condition is inserted.

Sometimes it is convenient to construct artificial problems by adding to a known potential some centrifugal terms, and sometimes such potentials arise naturally. We have seen the convenience of adding such a potential to the monopole problem, and later on we shall describe the results of making such a modification to the harmonic oscillator and Kepler potentials. In the case of the Dirac equation, the relativistic precession owes its existence to a naturally occurring term of this sort in the squared Dirac equation. It may happen that the centrifugal potential overwhelms the Coulomb potential in problems where they both are found together. The Coulomb potential predominates at long ranges, and so if it is attractive, there will result a bound region even for a repulsive centrifugal potential, which in turn predominates at short ranges. However, if the repulsive centrifugal potential is too large, the bound states may be lost, and if it is too attractive and counterbalances the natural centrifugal forces, the continuum we have mentioned may arise. This would occur for example in the Dirac equation for nuclei with charges greater than 137, although this is considerably beyond the limit of the heaviest nucleus now known. There has been some mention of such a possibility in the literature.

The unstable nature of the circular orbits in a centrifugal potential is matched by a similar situation in the field of a point electric dipole, wherein there exist semicircular orbits. Again, the slightest perturbations will cause these orbits to pass over into orbits which fall into the origin or recede to infinity. This point was responsible for some interesting discussions in the days of the old wave mechanics, when the mechanism of quantization of the radiation from atoms was still not well understood. Thompson (107) had proposed that atoms, which have a generally attractive central potential, but which could certainly be modified by an additional dipole if the charge were not symmetrically located at the nucleus, might possess electronic orbits in which the electron oscillated about a position of equilibrium off to one side of the atom. Such an oscillation depended upon the assumption that the semicircular orbits were stable, and that small displacements from them would result in bounded motion; the point was disputed in a rather interesting series of articles (108a-g) mostly by Higab (108d-f), in the *Philosophical Magazine* around 1930.

As for the case of the point dipole, it seems that if the dipole is finite, it is possible to have some bound orbits, which pass between the two nuclei. But, when one arrives at the limit of a pure dipole. if the dipole is not adequately strong, there can be no bound state.

The limiting case in the opposite direction is the Stark effect, in which one nucleus recedes to infinity as its charge grows, resulting in having a uniform field acting on the remaining nucleus. Redmond (109) has shown the connection of the separation constant in parabolic coordinates with the Runge vector, which we might compare with a rather similar relation found by Coulson and Joseph for the two-center problem. In the case of the Stark effect it is curious to note that if the energy is written in terms of the action-angle variables, one still finds a classical twofold degeneracy, which replaces the threefold degeneracy characteristic of the hydrogen atom. Since the threefold degeneracy is responsible for the accidental degeneracy of the spherically symmetric Coulomb potential, this residual twofold degeneracy should still result in accidental degeneracy in the cylindrically symmetric potential of the Stark effect. Bethe and Salpeter's *Handbuch* article (110) quotes results indicating that this degeneracy persists at least into the first orders of the quantum mechanical Stark effect.

As yet relatively little detailed investigation of the symmetry, possible ladder operators, and so on seem to have been made for the two-center problem or its limiting cases. Some other simple problems which likewise have not been much studied but which might show some interesting aspects are the motion of a charge particle in the field of an electromagnetic wave or a variant of the same theme which is to study the motion of a charged particle in the combination of a uniform magnetic field and an electromagnetic wave. In neither of these cases is either the symmetry or the degeneracy of the motion particularly known, although the orbits are reasonably regular.

## X Relativistic Systems

A final class of problems is composed of those involving relativistic motion, of which the most important member is Dirac's equation for an electron moving in a Coulomb potential. The most accurate analyses of the hydrogenic spectra show a fine structure, which is generally recognized as being relativistic in origin, which may be ascribed to the relativistic mass change of the electron as it moves from aphelion to perihelion with increasing velocity when one thinks in terms of the classical picture. In fact, Sommerfeld (111) had already in 1916 applied the old

quantum mechanics according to the Bohr quantization rules to obtain a fine-structure formula which coincided not only with the experimental observations, but also with the corresponding formula obtained over a decade later from Dirac's relativistic wave mechanical theory. The coincidence has always been considered rather remarkable, because the old quantum mechanics begins to break down rather badly when it has to treat many-body and relativistic problems. The confusion is no doubt due to the fact that Dirac's equation, as well as its rival, the Klein-Gordon equation, involves several rather distinct phenomena in a way which makes the mixture rather obscure. On the one hand, relativistic effects occur, but it would seem that these enter predominantly through the dependence of mass on velocity, although one should not slight the powerful influence of the requirements of Lorentz invariance and covariance. Rather independently of this, it seems that one cannot escape the necessity of using a multiple-component wave equation, or, in other words, a spinor field, to describe particles such as the electron. Relativistic considerations enter to determine the number of spinor components, and their transformation properties, but do not of themselves require the occurrence of a multicomponent wave function.

To see how relativistic effects enter in at the classical level, it is instructive to review Sommerfeld's derivation of the fine structure formula, phrased in Hamiltonian terms as it is done in Born's *The Mechanics of the Atom* (112). The relativistic Hamiltonian for the Coulomb problem is

$$\mathcal{H} = m \left( \left[ 1 + \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) \right]^{1/2} - 1 \right) - \frac{Ze^2}{r},$$

which is rather an awkward expression to use because of the occurrence of the square root of the momentum. For example, in the Hamilton-Jacobi equation, the derivatives of the principal function would be entangled in a manner which would make solution of the equation difficult. For this reason it is convenient to perform the algebraic manipulations necessary to remove the radicals, at the price of obtaining an implicit dependence of the resulting expression on the energy,  $W$ . We might call the resulting expressions the "squared" Hamiltonian:

$$\frac{1}{2m} (p_x^2 + p_y^2 + p_z^2) = W + \frac{Ze^2}{r} + \frac{1}{2m} \left( W + \frac{Ze^2}{r} \right)^2,$$

Nevertheless, when the time-dependence has been removed from the Hamilton-Jacobi equation through the introduction of the energy constant  $W$ , the resulting expression bears many resemblances to the nonrelativistic form of the hydrogenic Hamiltonian. Apart from a renormalization of the energy and of the electric charge arising from the implicit dependence on the energy constant which Sommerfeld noted as the relativistic modification of circular orbits, the principal new feature is the occurrence of a centrifugal potential  $Z^2 e^4 / 2mr^2$ , which is responsible for the orbital precession.

If one's only interest is in studying hydrogen atoms, one is likely to have to accept the ruination of the accidental degeneracy of the hydrogen atom thereby occasioned, since the Runge vector can no longer be a constant of the motion. However, if one's interest is in studying accidentally degenerate systems, irrespective of their physical reality, it is clear that the degeneracy may be restored by canceling the centrifugal potential. In fact this is the way

in which we proceeded earlier in producing a degenerate version of the magnetic monopole problem.

Here, however, one's freedom is more circumscribed, because the original Hamiltonian ought to be adjusted, and not the equivalent "squared" Hamiltonian. Sadly, the addition of a canceling centrifugal potential in the original Hamiltonian will produce inverse third and fourth powers of the radius as well as the inverse-square potential destined to cancel the term of relativistic origin. An attempt to cancel these new terms in their turn will lead to an infinite series, from which it does not appear possible to exclude an energy dependence. Alternatively we may have recourse to a vector potential to effect the desired adjustment. This potential must have a length equal to the centrifugal term, and be orthogonal to the momentum if no residual velocity-dependent terms are to appear; such a choice is  $A = Ze\hat{\ell}/r$ , where  $\hat{\ell}$  is a unit vector in the direction of the angular momentum. The resulting Hamiltonian,

$$\mathcal{H} = m \left( \left[ 1 + \frac{1}{2m} \left( \mathbf{p} - Ze^2 \frac{\hat{\ell}}{r} \right)^2 \right]^{1/2} - 1 \right) - \frac{Ze^2}{r},$$

is thus one whose relativistic orbits, including a precession due to the relativistic mass change, are just the Keplerian ellipses, although there remains a renormalization of energy and nuclear charge. It is therefore a relativistic system with the  $O(4)$  symmetry associated with the nonrelativistic hydrogen atom.

As for the hydrogen atom itself, a proper understanding had to await Dirac's equation, whose symmetry properties unfortunately seem to have remained obscure long after its other characteristics had become established. This has been due to the fact that Dirac's equation is in reality a very complex structure, whose properties have only gradually unfolded, even with a lapse of 40 years. When it was first enunciated, it showed so many unusual and paradoxical aspects, that it was hardly possible to know where to begin with its interpretation. Its acceptance, aside from the aesthetic aspect of its being a relativistically covariant equation, rested on its success in predicting the electron spin, and its yielding the experimentally acceptable value for the fine structure of the hydrogen spectrum. Its explanation of the electron spin was an outstanding accomplishment, for this quantity had seemingly come from nowhere, yet demanded to be taken into account in the interpretation of atomic spectra. Its ability to predict the fine structure correctly was no less impressive, for the failure in precisely this aspect had discredited Schrödinger's original relativistic wave equation, which has come to be called the Klein-Gordon equation, and had inspired Dirac's search for a more adequate relativistic wave equation in the first place, as well as having impeded Schrödinger's original formulation of wave mechanics.

In spite of its impressive and unflinching success in predicting the energy levels and probability distributions for numerous quantum mechanical systems, one began to encounter philosophical and practical difficulties with the Dirac equation almost at once. Part of the complexity of the Dirac equation is due to the fact that it is a first-order and not a second-order differential equation. Group invariants as applied to quantum mechanical problems are generally quadratic in the coordinates and momenta; we think of such things as the square of the radius, or the kinetic energy operator which is the square of the momentum vector, in the case of the rotation group, or the form  $(r^2 - t^2)$  preserved by the Lorentz group. Such expressions are readily converted into differential operators, whereas such functions of them

as their square root are not. Moreover, the Dirac Hamiltonian derives its fame precisely from *not* being the square root of an invariant operator expression, but rather from being a hypercomplex operator, free of radicals, whose square results in such an invariant expression. Herein lies the hidden assumption of a multicomponent wave function, and the eventual complication that along with the infinitesimal transformations of space-time operators there must be incorporated operators mixing the components, if one hopes to produce invariant expressions. Such behavior is characteristic of any field theory, and we should recollect that even the Maxwell equations do not lead to spherical symmetry and conservation of angular momentum until account is taken of the angular momentum which may reside in the field itself.

Dirac therefore started from the relativistic energy of a free particle

$$\mathbf{E}^2 = \mathbf{p}^2 + m^2$$

and postulated that there existed a hypercomplex operator of the form

$$\mathcal{H} = \alpha \cdot \mathbf{p} + \beta m,$$

the square of which would result in the ordinary expression for the energy. To obtain such a result one must require that the operators  $\alpha_i$ , satisfy the relationships

$$\begin{aligned} \alpha_i \alpha_k + \alpha_k \alpha_i &= 2\delta_{ik}, \\ \alpha_i \beta + \beta \alpha_i &= 0, \\ \beta^2 &= 1. \end{aligned}$$

In other words, it is necessary to have a set of four anticommuting operators, whose squares are unity. The representation theory of hypercomplex numbers shows that there is only one faithful irreducible matrix representation of such a set of operators, and that this representation requires the use of 4 x 4 matrices – the so-called Dirac matrices. As a result the number of components of an irreducible wave equation is likewise four, a result depending on the requirements for a set of four mutually anticommuting matrices and thus only very indirectly related to the four dimensionality of Minkowskian space-time.

One ought to take note of several features of the assumptions involved in the formulation of the Dirac equation. The decision has been made to work with a multicomponent wave equation, and moreover that it is to assume a Hamiltonian form through the relativistic formula for the energy of a free particle. However, the operator to be used as a Hamiltonian is one whose square yields the relativistic energy, squared, in order that it itself may depend linearly on the momentum. This necessitates the intrusion of anticommuting operators; but there is an explicit assumption that the space-time operators such as the position and momentum, and the hypercomplex anticommuting operators, are cleanly separated, as it were. In other words, we are assuming that the use of a multicomponent wave function, with the space-time operators, and especially the momentum operators, acting on the various components of the wave function individually is an adequate way to avoid the square-root operators which would occur in a more straightforward transcription of the relativistic Hamiltonian into operator form. That such an arrangement actually bears fruit must be regarded as really rather remarkable, but at the same time one must clearly understand that there are two effects involved. One is that the equation is a proper relativistic equation, and so must be expected to take relativistic effects into account as an automatic consequence of its formulation. However, the other, equally important hypothesis is that of a multicomponent wave function.

Whatever the philosophical or metaphysical origin of the Dirac equation, once its usage is agreed upon, it is nothing but a set of first-order linear differential equations, to which the ordinary mathematical reasoning concerning symmetry and invariance must apply, just as any other properties of the solutions might be discussed. In this regard, the first observation which may be made is that this set of equations is not even rotationally or reflectionally invariant. From the original Hamiltonian  $\mathcal{H} = [\alpha \cdot \mathbf{p} + \beta m]$  inversion in the origin produces  $\mathcal{H} = [-\alpha \cdot \mathbf{p} + \beta m]$  while a rotation produces the Hamiltonian  $\mathcal{H} = [\alpha \cdot \mathbf{p}' + \beta m]$ , where  $\mathbf{p}' = R(\mathbf{p})$  is the rotated momentum and therefore most certainly a different vector from the original.

Since one has the intention of using Hamiltonian mechanics in its accepted form, albeit in a formal way, and even though this Hamiltonian is now thought of as a hypercomplex number, it is convenient to define the orbital angular momentum in terms of the canonical momentum in the accustomed way,

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

and to calculate its commutator with respect to the Dirac Hamiltonian. As is to be expected from the lack of manifest spherical symmetry of the Dirac Hamiltonian, one finds at once that the orbital angular momentum is not a constant of the motion; in fact its derivative is  $-i\alpha \times \mathbf{p}$ . After a certain amount of trial and error it is readily enough found that there is another “vectorial” quantity

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$$

( $\alpha = \rho_1 \boldsymbol{\sigma}$ , in Dirac’s notation) whose time derivative is the negative of that of the orbital angular momentum, justifying the introduction of the “total” angular momentum

$$\mathbf{J} = \mathbf{L} + \frac{1}{2}\boldsymbol{\sigma}$$

as a constant of the motion, and referring to this other quantity as the “spin” angular momentum. Historically, its discovery was no great accident, for the electron spin was well known, and one of the major successes of the Dirac equation was just the fact that its inclusion in the conserved total angular momentum was imperative. Mathematically speaking, it is seen that the spin is a direct consequence of the multicomponent wave function, for the simple reason that a rotation of a wave not only alters the way in which the wave components depend on the coordinates of the space, but it also reorganizes the way in which they are recognized as components belonging to the various coordinates. The rotation of coordinates is done by the orbital angular momentum, while the reorganization of the components is done by the spin angular momentum. In this way a Dirac particle acquires an “intrinsic” angular momentum, but it must be understood that the spin angular momentum exists exclusively to relabel the four components of the multicomponent Dirac wave function. Since the Dirac Hamiltonian has the formal structure of an inner product, one can also understand the symmetry in terms of a simultaneous rotation in the two spaces joined by the inner product.

Thus the spin of the Dirac electron, while indirectly of relativistic origin, is primarily a consequence of the use of a multicomponent wave function. Galindo and Sánchez del R  o (113) have emphasized this point by showing that a multicomponent Galilean invariant theory can also be constructed, in which a spin nevertheless makes its appearance. L  vy-Leblond (114) has examined such a theory exhaustively. The secondary effects of relativity, which have their Galilean counterparts, and which in fact do influence the spin, have to do with the number of components required for the spin functions, which depends on the dimension of

Minkowski space. In turn, this determines the precise numerical value of the spin, as well as the transformation properties of the spinors with respect to rotations, or even more general Lorentz transformations.

## XI Zitterbewegung

Relativity and spinorial properties are not the only obstreperous features of the Dirac equation, as one discovers when he begins to obtain explicit solutions and to delve further into the properties of that equation.

Taken at their face value, the Hamiltonian equations tell us that

$$\dot{\mathbf{x}} = [\mathcal{H}, x] = \alpha.$$

In other words, the velocity is determined by an operator for which it can be shown that the only eigenvalues are  $\pm 1$ , and such that moreover the different velocity components do not commute. This result is very much at variance with our nonrelativistic and even classical relativistic experience. No particle may move at the velocity of light, and moreover, we expect any velocity component to be possible in the entire open interval between  $-1$  and  $+1$ . Perhaps the difficulty lies in the construction of pure states, and that in practice we only see a packet combining several of the pure states, with the electron darting in every which direction.

Whatever its origin, the difficulty is real enough, and has been known from the beginning of the theory of the Dirac electron. It was Breit (115) who first noticed the anomaly in the velocity operator in 1928, and Schrödinger (116) who integrated the equations of motion two years later to obtain

$$x_k(t) = x_k(0) + p_k \mathcal{H}^{-1} t + \frac{1}{2} i (\alpha_k(0) - p_k \mathcal{H}^{-1}) \mathcal{H}^{-1} e^{-2i\mathcal{H}t}.$$

Here it is to be seen that the position operator consists, as we would expect, of the sum of an initial position vector, a displacement which is proportional to the elapsed time, and finally an unexpected term which represents a violent oscillation of the particle with an amplitude equal to its Compton wavelength. This latter motion has come to be known as the “*Zitterbewegung*” of the electron. Breit, Schrödinger, and Fock each contributed some further insight into the necessary interpretation for this kind of motion. It served nicely to attribute a geometrical extension to what otherwise would have had to have been regarded as a point particle, but it was also clear that there were things which were out of the ordinary in the motion of such a particle. Such behavior can also be explained, or at least the possibility can be rendered plausible, on the basis of a multicomponent wave function. Since it requires four separate wave functions to determine the position of a particle, it could very well happen that through some intrinsic property of the Dirac Hamiltonian all four components of the wave function could never concentrate in the same spot, or to say the same thing in another way, it could very well happen that the four components could always interfere in such a way that the particle could never be localized beyond a certain optimum.

A rigorous demonstration of just such a limitation was found in 1950 by Foldy and Wouthuysen (117) as a result of trying to separate positive and negative energy solutions of the Dirac equation, and by Newton and Wigner (118) while trying to establish the optimum localizability of a particle if the wave functions were confined to those belonging to



energies of only one sign. In other words, of the four components of the Dirac wave function, the interference can be attributed principally to one pair of positive energy components interfering with the other pair of negative energy. Understanding of the phenomenon depends upon the way in which we can attribute some individual significance to the four components of the wave function, and this in turn is rather closely related to the behavior of these same components in the nonrelativistic limit.

The primary subdivision of importance is that into positive and negative energy components, which is to a certain extent related to the occurrence of the square root in the relativistic energy formula, which could have either sign. Classically, a particle for which one sign is chosen will move in such a way that the sign is fixed, for no motion is possible which would make the radicand zero, and thus no transition to the other sign could occur.

Although the Dirac Hamiltonian is ostensibly free of any square roots, this freedom has been bought at the price of a multicomponent wave function and anticommuting hypercomplex operators. It is known that if invertible operators anticommute, their eigenvalues must occur in negative pairs. In particular, if an operator can be found anticommuting with the Dirac Hamiltonian, the latter must have eigenvalues of both signs. For the free particle such an operator exists; it is  $\beta$ , and thus there must be wave functions of both signs of the energy.

Not only does the presence of an anticommuting operator necessitate negative eigenvalue pairs, but if one of the operators is partially diagonalized, the other must be brought to skew diagonal form by the same transformation. Unfortunately the converse is not entirely true; bringing one operator to the skew diagonal form will not necessarily diagonalize the other. Let us call a partially diagonal operator an “even” operator and a skew-diagonal operator an “odd” operator. The essence of the paper of Foldy and Wouthuysen was to show how one could construct a transformation which would bring a large class of Dirac Hamiltonians to even form. Postulating a transformation of the form

$$\mathcal{H}' = e^{i\mathcal{A}}\mathcal{H}e^{-i\mathcal{A}},$$

where the logarithm  $\mathcal{A}$  is assumed to have the general structure

$$\mathcal{A} = \frac{i}{2m}\beta\alpha \cdot \mathbf{p}\varphi$$

with  $\varphi = \varphi(p/m)$ , an as yet undetermined operator (which commutes with  $\alpha$  and  $p$ ), one finds that the transformed Hamiltonian becomes

$$\mathcal{H}' = \beta \left[ m \cos \frac{p\varphi}{m} + p \sin \frac{p\varphi}{m} \right] + \alpha \cdot \mathbf{p}p^{-1} \left[ p \cos \frac{p\varphi}{m} - m \sin \frac{p\varphi}{m} \right].$$

Then, the choice

$$\varphi = (\arctan p/m)/(p/m)$$

would result in the desired transformation to even form.

The important point about the application of the Foldy-Wouthuysen transformation to the Dirac Hamiltonian of a free particle is that it results in a separation of the positive and negative energy states, as can be seen from the form into which it transforms the Hamiltonian, which is curiously enough the classical relativistic energy operator multiplying the diagonal operator  $\beta$  (in the usual representation),

$$\mathcal{H} = \beta\sqrt{\mathbf{p}^2 + m^2}.$$

One could discuss at some length the selection of the most appropriate operators for use in relativistic wave mechanics. The energy radical which is the naive choice for the relativistic Hamiltonian operator is in fact the Dirac Hamiltonian in the Foldy-Wouthuysen representation, multiplied by the operator  $\beta$ . When it is applied to the coordinate operator by taking the commutator bracket, as time derivatives are generally obtained, so as to obtain the velocity operator, the result is the transform of an intuitively acceptable quantity. Thus, one could almost think that the paradoxes of the Dirac equation are the result of nothing more than a choice of representation, and the insistence of a separation of space and spin. Such an attitude conceals the fact that the paradoxes arise from the multicomponent aspects of the theory, and a single-component theory does not, in fact, adequately represent the experimental facts. Such deficiencies are not too apparent in the theory of a free particle, even though in this simple case the negative energy states are already manifested, as well as the intrinsic angular momentum of the particle which the theory describes, neither of which show up in a single-particle theory.

There are other approaches to the Foldy-Wouthuysen transformation. Pryce (119) has shown that it is the transformation to a coordinate system in which the electron is at rest. It is difficult to form a relativistic theory of many particles, so that it is not entirely clear how to extend such a theory to a many-body system; for example, to find the relativistic center of mass transformation for a pair of particles interacting through a Coulomb field, Newton and Wigner have discussed the possibility of forming a localized wave packet from relativistically invariant wave functions, and have also been lead to the Foldy-Wouthuysen position operator.

Moreover, the Foldy-Wouthuysen transformation is only one of a general class of transformations which one can occasionally use advantageously to transform the Dirac equation. For example, the transformation of Cini-Touschek (120) may be used to place the Dirac Hamiltonian in a skew-diagonal form in circumstances similar to those in which the Foldy-Wouthuysen transformation places it in diagonal form. Their representation is useful for treating ultra-relativistic problems. In this region, the rest mass of the particle is negligible in comparison with its kinetic energy, and thus has as its limit the theory of a zero-mass particle, such as the neutrino. These possess symmetries and constants of the motion all their own.

In recent years there have been a considerable number of papers bearing on the Foldy-Wouthuysen transformation and its generalizations. One finds that nearly all the relativistic wave equations, even for higher spin particles, show similar difficulties due to the simultaneous presence of positive and negative energy solutions. Although the majority of these difficulties can only be removed by second quantization and the formulation of a quantum field theory, it is more the interpretation of probability densities and the positive definiteness requirements on the wave functions which finally force the adoption of such remedies, so that one can still obtain much valuable insight as well as practical results by a separation of the energy states in the first-quantized theory.

Inasmuch as the Foldy-Wouthuysen type of transformation resolves the existence of *Zitterbewegung* and related phenomena by attributing them to interference between the positive and negative energy waves, and separating the two types of wave functions, one may well wonder whether it is absolutely necessary to include both types of wave functions in the wave equation. Mathematically the answer is yes, because neither set of wave functions by itself is complete, in the sense of being able to manufacture arbitrary probability distributions in terms of them. Some physical evidence in this direction is provided by the fact that the Dirac equation can be written in the form of a second-order partial differential equation after

all. This formulation lacks the elegance of the Dirac first-order form because it requires an explicit introduction of a spin magnetic moment, which then becomes an *ad hoc* assumption. The possibility of writing the Dirac equation in this form has existed from the first, but it has lately been revived and applied to explain certain coupling in the weak interaction processes by Feynman and Gell-Mann (121) and additionally by Brown (122).

Second-order differential equations traditionally require negative pairs of eigenvalues in their solutions, if they obey relatively rudimentary symmetry requirements, such as showing time reversal symmetry. Such considerations may therefore lie behind the presence of solutions of the relativistic wave equations of both signs of the energy.

Quite independently of such abstract and theoretical considerations, however, the negative energy states have played a considerable role in the historical development of quantum mechanics because of a number of paradoxical physical manifestations of their existence. The most famous of these is perhaps the Klein's paradox, which occurs for a Dirac electron moving in a field with a very steep potential gradient; ideally this can simply be a potential step. For plane waves representing a free electron the two energy states are well separated, and if the negative energy states are initially unoccupied, they will forever remain so. When a perturbation is introduced, transitions can occur, with a catastrophic energy release, as the particle descends into more and more negative energy states. To preclude this from happening, Dirac invented the hypothesis of the negative electron sea and invoked the Pauli exclusion principle from many-particle theory. However, the potential step of the original Klein's paradox provides an exactly soluble problem in which, if such disastrous solutions do not quite occur, they still destroy the possibility of a discrete spectrum.

The literature of the early 1930s contains several papers which verify that similar difficulties occur in a number of other similar situations, for example, in the relativistic harmonic oscillator. In spite of the particle's apparently being bound in the ever-increasing harmonic oscillator potential, there are no bound states, and the negative energy components always have a non-negligible amplitude. Therefore, by the time that Foldy and Wouthuysen made their analysis, there was ample evidence that the role of the negative energy states in the Dirac equation needed clarification.

Thus, by 1950 there had emerged a fairly clear idea of the significance of the four components of the Dirac wave equation, that they corresponded to the occurrence of two energy states and two spin states, and some of the complications which their existence could produce. *Zitterbewegung* owed its origin to the interference between the positive and negative energy states, primarily, while spin arose from the fact that a rotation of configuration space resulted in a mixing of the components of the wave function.

## XII Dirac Equation for the Hydrogen Atom

Interesting as the solutions of Dirac's equations may be for plane waves, and even for the motion of a charged particle in a uniform magnetic field, it is in the treatment of the hydrogen atom that the equations show their true utility, and also where they have resisted for the longest time the analysis of their symmetry. This recalcitrance was apparent from the start, for rigorous solutions to the equations for the hydrogen atom were not obtained until after some of the simpler systems had first been considered, and it was verified that the magnetic moment of the electron arose as a natural consequence of this type of wave equation. However,

once the hydrogenic equation was analyzed, operational techniques were applied from the very beginning, along with more traditional methods of series solution. Such methods may be found in the early papers of Temple (123), in his small monograph (124) on quantum mechanics, as well as in some contemporary publications of Sauter (125).

On trying to construct a relativistic wave equation for systems in which there are interactions between various particles, the first approach is the usual one, to assume that the particles interact through fields, and that one may therefore to a first approximation treat the motion of a single particle in a fixed field, the most important being the electromagnetic field. The electromagnetic field may be introduced into Hamiltonian mechanics by adding the vector potential to the canonical momentum, but if one is to follow relativistic analogy in its entirety, the electrostatic field ought to be added to the Hamiltonian as well since it represents the fourth component of a vector in Minkowski space. In that way the Dirac equation may be formulated for the relativistic hydrogen atom, choosing a Lorentz frame in which the potential is purely electrostatic.

Although the Dirac equation is a *covariant* equation with respect to general Lorentz transformations, which means that the transformation rules for vectors are to be used in converting it from one coordinate system to another, when it is applied to a specific example such as the hydrogen atom which has spherical symmetry, one should expect to find an *invariance* to rotations.

However, for the same reasons that we have described, concerning the plane wave, the fact that we are dealing with a first-order system of equations and not with differential operators formed from group invariants precludes our finding such a symmetry. Here also we find that a rotation of the spatial coordinates must be coupled with a simultaneous mixing of the spin components, with the result that again it is the total angular momentum which is the conserved quantity and which generates a symmetry transformation. The orbital angular momentum by itself is not conserved, which implies the existence of a spin angular momentum in the Coulomb potential as well as for the free particle.

On account of the precession of the hydrogenic orbits in relativistic classical mechanics, one does not really expect to find that the Runge vector is a constant of the motion of the Dirac equation, nor that the accidental degeneracy of the hydrogen atom remains. This loss of degeneracy is in accord with the experimentally observed hydrogenic spectrum, and is confirmed by the solutions of the Dirac equation, which give very close agreement with the results. Perhaps for this reason symmetry considerations have never been pushed very far for the Dirac equation of the hydrogen atom, but there nevertheless remains a very mysterious two-fold degeneracy, above and beyond the degeneracy which one would expect from the spherical symmetry and the conservation of the total angular momentum. This degeneracy seems to be characteristic of the Dirac equation, but not of the Klein-Gordon equations, and is not uniquely confined to the Coulomb potential as had sometimes been thought. We shall see that it depends on the existence of the spin angular momentum, and represents a degeneracy in what might be called the “helicity” of the Dirac wave functions.

The Dirac equation for the Coulomb potential has the form

$$\mathcal{H}(m)\Psi = \left( \alpha \cdot \mathbf{p} + \beta m - \frac{\alpha Z}{r} \right) \Psi = -E \Psi.$$

However, the usual method for solving the Dirac equation is to construct the mass annihilation

operators

$$\begin{aligned}\mathcal{O}_+ &= \rho_3[\mathcal{H}(m) + E], \\ \mathcal{O}_- &= \rho_3[\mathcal{H}(-m) + E],\end{aligned}$$

and to observe that any solution of the Dirac equation must also be a solution of the “squared” equation

$$\mathcal{O}_+\mathcal{O}_-\Psi = 0,$$

which in the present instance takes the form, written in polar coordinates

$$\left[ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{K^2 - (\alpha Z)^2}{r^2} - \frac{2\alpha Z E}{r} + \frac{1}{r^2} (\rho_3 K + i\alpha Z \rho_1 \sigma \cdot \hat{\mathbf{r}}) + K^2 \right] \Psi = 0,$$

where  $K = \rho_3(\sigma \cdot \mathbf{L} + 1)$ .

Here, the role played by two terms is to be noticed. The term  $(K^2 - (Z\alpha)^2)$  may be thought of as a term in the square of the angular momentum causing a relativistic precession by slightly splitting the energy of the different states of a given total angular momentum. This term appears in the Klein-Gordon equation, but does not give the experimental amount of fine structure splitting.

That it does not do so is due to the term dependent on

$$\Gamma = \rho_3 K + i\alpha Z \rho_1 \sigma \cdot \hat{\mathbf{r}}.$$

In fact, if the equation is rewritten in terms of  $\Gamma$ , it acquires the very suggestive form

$$\left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{\Gamma(\Gamma - 1)}{r^2} - \frac{2k\eta}{r} + k^2 \right) \Psi = 0,$$

where  $k^2 = E^2 - m^2$ , and  $\eta = \alpha Z E/k$ .

As a first remark, let us say that the operator  $K$  occupies a role quite similar to the angular momentum operator, and in fact has eigenvalues which are substantially the eigenvalues of the total angular momentum. It may be demonstrated to be a constant of the motion, whose eigenvalues may be used to classify the quantum states of the wave functions. In fact, the twofold accidental degeneracy of the Coulomb potential arises out of the fact that the energy depends only upon the absolute value of the eigenvalues of  $K$ , whereas wave functions occur belonging to eigenvalues of  $K$  of both signs. For a long time, only  $\mathbf{J}$ ,  $\mathbf{J}^2$  and  $K$  were known as constants of the motion, leaving open the possibility for speculation as to what other constant of the motion might exist that would be responsible for the additional degeneracy. Such a constant was found in 1950 by Johnson and Lippman (126), with the interesting property that it commuted with the Hamiltonian, but anticommuted with  $K$ . It therefore simultaneously forced  $K$  to have negative pairs of eigenvalues, and made them degenerate in energy.

Johnson and Lippman’s constant probably exists for all spherically symmetric potentials, and certainly does so for a plane wave, where it measures the projection of the spin on the momentum of the particle. For the Coulomb potential, it seems to correspond more nearly to the projection of the spin on the Runge vector, but in any event its physical significance seems to be that it determines the relative orientation of the spin and some reference vector in the system.

Several methods exist for solving the squared Dirac equation, of which some noteworthy instances are the methods of Hylleraas (127) and Kolsrud (128). One version of considerable historical antiquity is simply to determine the eigenfunctions of the operator  $K$ , which correspond to the angular part of the equation. They are not difficult to determine, inasmuch as they are the same spin functions which had arisen earlier in Pauli's theory of the spinning electron. Once the angular part of the equation is separated, there remain some coupled equations for the radial functions, whose resolution by various schemes forms the substance of the various papers mentioned above. One of the more comprehensive recent treatments was made by Martin and Glauber (72), and later extended by Biedenharn (130).

Biedenharn's proposal was to diagonalize the operator  $\Gamma$ , which may be accomplished by a Foldy-Wouthuysen transformation applying only to  $\Gamma$  and not to the entire Hamiltonian. It was found that the radial wave functions occurring in such a representation were exactly like the nonrelativistic Coulomb wave functions, with the difference that the eigenfunctions of angular momentum which are half-integers or integers in the nonrelativistic treatments are modified by the fine structure. In other words, there resulted a considerably simplified way of obtaining the radial wave functions of the Coulomb problem.

As we have already explained in connection with the description of the magnetic monopole problem, it can often be quite instructive to consider an alternative system which might not be physically realistic, but which nevertheless might have some exceptional property worthy of study, such as an extraordinarily high degree of symmetry. A similar idea occurred to Biedenharn, to modify the Coulomb problem in such a way as to obtain a degenerate Hamiltonian, if possible one which retained the nonrelativistic degeneracy of the hydrogen atom. We have already seen that there exists such a related classical Hamiltonian, which not only has the same degeneracy but the same symmetry group. The modification which suggests itself is simply to replace the operator  $\Gamma$  by an operator having desired eigenvalues, such as  $K$  itself. However, the framework of the Dirac equation requires this to be done with considerable finesse, for the alternative system which we hope to obtain is to be described by a modified Dirac Hamiltonian, and not by a modification in the squared equation. Thus, a modification which is readily apparent in the squared Hamiltonian will require some ingenuity to take account of the noncommutation of quantum mechanical operators and the functional dependence of the squared Hamiltonian on the original Hamiltonian.

Nevertheless, Biedenharn (131) succeeded in discovering the term which was necessary to add to the Coulomb Hamiltonian,

$$\mathcal{H}_{fs} = \rho_2 \frac{\boldsymbol{\sigma} \cdot \hat{\mathbf{r}}}{r} K \left( \left[ 1 + \left( \frac{\alpha Z}{K} \right)^2 \right]^{1/2} - 1 \right)$$

and another Foldy-Wouthuysen transformation which diagonalized the angular momentum term in the resulting squared Hamiltonian. The details were set forth by Biedenharn and Swamy (132), in the paper in which they introduced their "symmetric" Hamiltonian.

Sheth (133), in 1968, took the Foldy-Wouthuysen nonrelativistic limit of the symmetric Hamiltonian, to see that it approaches the Hamiltonian we mentioned in the introduction to this section, in which the relativistic precession is canceled by a vector potential whose magnetic field causes a counterprecession. It is worthy of note that there are two relativistic effects which occur in the orbital precession of the hydrogenic orbits. One is, let us say, an average mass deviation which we could attribute to the relativistic mass change a particle

moving at the average orbital velocity would experience. It would even be possible to interpret this effect in terms of a modified central nuclear charge rather than in terms of a mass variation of the electron. This is the variation which Sommerfeld called the relativistic correction for circular orbits. Additionally, there is the further mass variation which changes with the particle's position in the orbit, and which leads to the precession. This division of the relativistic effects into two parts affects the nature of the approximations which one might use in calculating the relativistic Coulomb wave functions. Biedenharn and Swamy found that the perturbation series which would result from removing the fine structure interaction from the symmetric Hamiltonian was not quite the same series which was found by Furry, Sommerfeld and Maue (134), Bethe and Maximon (135), and others who were concerned with incorporating relativistic effects into the Coulomb wave functions through series expansions.

The symmetric Hamiltonian shows  $O(4)$  degeneracy, and it is apparent that the angular momentum and the Runge vector are constants of the motion generating this degeneracy when an appropriate coordinate system is used. To exhibit these constants in the customary Dirac representation is a relatively cumbersome task, but in any event, Biedenharn and Swamy did exhibit a set of operators generating the  $O(4)$  group in their paper.

Even in the symmetric Hamiltonian, the complete degeneracy is not merely the  $n^2$  degeneracy of the group  $O(4)$ , but it is  $2n^2$ , double the expected amount. Again it is found that there is a twofold  $K$  degeneracy. Its presence can be explained by an operator which, like the Johnson-Lippmann operator, is a constant of the motion and anticommutes with  $K$ . Whereas Biedenharn and Swamy showed that their symmetric Hamiltonian has two vector constants of the motion generating an  $O(4)$  symmetry group, the symmetry is not as simple as it appears. Although the total degeneracy is  $2n^2$ , it arises from the accidental degeneracy of a representation of dimension  $n(n+1)$  of  $O(4)$  with one of dimension  $(n-1)n$ , so that one has not found a degeneracy which could have an interpretation in terms of wave functions defined on a hypersphere.

In the most delicate experiments, it is found that not even the  $K$  degeneracy occurs, the very small difference in energy between these levels which occurs being the Lamb shift, which was measured precisely enough to establish the nondegeneracy with certainty in 1948. However, it is due to effects not treated at the level of approximation of the Dirac equation – interaction of the electron, with a quantized radiation field being the essential omission.

### XIII Other Possible Systems and Symmetries

Of the relativistic systems which have been treated by Dirac's equation, the ones we have already mentioned are by far the most important. These are the motion of a free particle, the motion of a charged particle in a uniform magnetic field, and finally, the relativistic hydrogen atom. However, there are a handful of other problems which have also received some consideration, but which show symmetry or degeneracy to an even lesser extent than those which we have already described, which was already very little. The motion of a particle in a uniform electric field was investigated to clarify Klein's paradox, by Sauter (136) in 1931. Klein (137) had published his own treatment of the motion of a particle across a potential step two years earlier, while there was an investigation of the harmonic oscillator potential also motivated by Klein's paradox by Nikolsky (138) in 1930 and a later commentary by Postepska (139) in 1935. Sommerfeld and Welker (140) studied a truncated Coulomb potential in 1928. Even in

the nonrelativistic realm, the tunneling of particles through potential barriers had been investigated. Von Neumann and Wigner (141) studied a system in which the apparently localized states were embedded in a continuum, and it was known that one had to take similar possibilities into consideration in dealing with exceptionally strong Stark effects for the hydrogen atom, which has a certain probability of spontaneous ionization in such circumstances. The relativistic examples were mainly interesting because the tunneling occurred to the negative mass states.

As a certain generalization of the motion of a particle in a uniform magnetic field, it was found that the equations were also soluble for motion in the field of a plane electromagnetic wave, as well as for some combinations of electromagnetic waves and static fields. Stanciu (142) has found some additional exactly soluble potentials within the last few years.

Turning to other kinds of generalizations, there has been a little if not much interest in the solution of Dirac's equation in spaces of different dimensionality than the familiar space-time. Ionesco-Pallas (143) has solved the Dirac equations for a two-dimensional hydrogen atom, while Coulson and Joseph (144) have discussed the extension of the Dirac equation to  $n$  dimensions, and seen that the general treatment is applicable to three dimensions. Cartan, in his theory of spinors, also discussed the extension of the Dirac equation to many dimensions. Of course, there have been numerous attempts to place the Dirac equation in the framework of general relativity, or write it in various degrees of abstraction using differential geometry or the algebra of hypercomplex numbers.

One ought to be a little cautious in speaking of the  $n$ -dimensional hydrogen atom, because all such discussions tend to take the appropriate potential as  $1/r$ , as it is in three dimensions. However, it is only in three dimensions that this is the potential which permits the application of Gauss' law, so that a potential arising in a space of different dimension would more than likely have a different dependence on the radius. The reason that the assumption of  $1/r$  as a potential is generally made is that it leads to a degenerate energy spectrum, thanks to the fact that the angular frequency of the radial action angle variable is compatible with the angular variable in classical mechanical problems of whatsoever dimension, when the potential  $1/r$  is uniformly used for all dimensions.

Except insofar as we have mentioned the Klein-Gordon equation for the hydrogen atom in passing, we also have not mentioned the symmetry properties of possible relativistic or Galilean wave equations for particles of higher spin. This is a topic which is rarely carried to the extent even of solving the equations for a hydrogen atom. There remains one further avenue of possible generalization, which is to consider the possibility of more general invariance groups than the Lorentz group. There is ample historical precedent for such an extension, as it was found in 1910 that Maxwell's equations are invariant under the conformal group, which includes the Lorentz group as a subgroup. The principal additional symmetry operations which it includes allow one to view the universe in a mirror expanding at the velocity of light, as well as from a rotated or uniformly moving coordinate frame. Combinations of such transformations would require invariance under dilations as well as the other Lorentz transformations.

The application of the conformal group to physical systems has never achieved the popularity that the Lorentz group has, principally because of the difficulty in finding a mechanical interpretation of its consequences, as typified by the relativistic mass increase, the time dilation or Lorentz contraction, or the mass-energy equivalence formula. In fact, it seems that forces would have to depend on third rather than second derivatives, to allow the experimental



indistinguishability of different reference frames connected by conformal transformations.

On the other hand, there is still the conformal invariance of the Maxwell equations, and the Dirac equation for zero-mass particles, to suggest that conformal invariance might still have some physical role to play. Should such an influence exist, it would only be through the form of the basic equations of physics, and would not enhance the spherical symmetry of systems such as the hydrogen atom, unless it were possible to attribute the accidental degeneracy of the hydrogen atom to the conformal group as a direct consequence of the conformal invariance of some specific equations of motion. For example, even though the Dirac equation of the hydrogen atom is formulated in a relativistically invariant theory, we have seen that it nevertheless loses its accidental degeneracy, and that although it retains its spherical symmetry, it does not gain a Lorentzian symmetry.

Possible interest in the conformal group exists because of the appearance in recent years of a vast amount of experimental evidence concerning the elementary particles, together with all the indications of a very extensive amount of symmetry. Up until the past half decade, not only the conformal group, but the entire subject of accidental degeneracy and its connection to particle mechanics has remained a relatively esoteric subject, with its only major application being to nuclear shell theory. Perhaps just because of its success in this latter realm, it suddenly attracted widespread interest as a means of organizing the theory of elementary particles. There has long been a feeling that perhaps we have not understood nature's symmetry to the fullest. Just as the deepest understanding which we now have of quantum electrodynamics came as a result of casting the theory in a relativistically invariant form, there has been considerable speculation that either the conformal group or some extension of the Lorentz group arising from general relativity might lead to a further broadening of our physical understanding. Whatever merits there might be to search for further symmetry in nature, there was the undeniable phenomenological success of the attempt to classify the elementary particles according to the irreducible representations of more and more general groups,  $O(4)$ ,  $SU(3)$ ,  $SU(6)$ , and many others, even though none of these symmetry groups has been entirely satisfactory, and even though none of them seem related to the dynamical symmetry of some equation of motion.

The attempt to enlist the conformal group has met grave difficulties. Although Maxwell's equations are conformally invariant, and indeed this was the source from which this group first came to the attention of physicists, it has not been possible to secure an attractive interpretation of conformal invariance in other branches of physics, particularly mechanics. In any event the conformal group is not compact, but only locally compact, with the result that all its irreducible unitary representations are infinite dimensional, and hence not directly related to the occurrence of finite accidental degeneracies among bound states.

Nevertheless, the conformal group does have one interesting connection with the accidental degeneracy of the hydrogen atom. In Fock's representation, let us say for the bound states, the energy surfaces are hyperspheres of radius depending upon the energy, and the Keplerian motion is equivalent to force-free motion on the hyperspherical surfaces. Now, the conformal group is just precisely that group which maps spheres into spheres, so that some of its transformations ought to be symmetry operations for the hydrogen atom (namely, the four-dimensional rotations), and others of them ought to map states of one energy into states of another energy.

There is an extensive lore of the theory of ladder operators which transform wave functions with certain quantum numbers into others with different quantum numbers. Sometimes the

theory has been connected with group theory, as in the case of angular momentum ladder operators, and sometimes it has been formulated in an entirely independent manner, as it was in a series of researches culminating with the paper of Infeld and Hull (145) in 1951, which contains an extensive bibliography of previous work on the subject. Needless to say, there have been other attempts to unify the two approaches (146).

Investigation has shown that the conformal group is indeed related to the spectrum of the hydrogen atom, in such a way that the entire bound state spectrum is subsumed in one single irreducible representation of the conformal group. In the most general case, an irreducible representation of a group will reduce into several irreducible representations of a subgroup. In the case of the conformal group, there exists an irreducible representation which contains each of the  $n^2$  dimensional representations of the  $O(4)$  group exactly once, and such that the bound state wave functions of the hydrogen atom form a basis for this representation. Of course, the hydrogen atom Hamiltonian will not commute with the generators of such a group which lie outside the Lie algebra of generators of the  $O(4)$  symmetry group, but the remaining generators are found to be the energy ladder operators of the hydrogen atom. Thus, we have another instance of the existence of a family of operators which determine the shape of the spectrum of the Hamiltonian as well as its degeneracies. In 1966 Hwa and Nuyts (147) showed that similar groups exist encompassing the states of the harmonic oscillator. Such groups have come to be called *noninvariance* groups and are characterized by the fact that their generators do not necessarily commute with the Hamiltonian, but are eigenfunctions of the Hamiltonian with respect to the operation of commutator bracket. That is, they satisfy the commutator equation which is the requirement that they in turn act like ladder operators for the Hamiltonian. One of the earliest applications of such relationships in physics was by Goshen and Lipkin (58), but they were also used by Schwinger (148) for harmonic oscillator operators in his theory of angular momentum,

The recent search for noninvariance groups and higher symmetry groups has clarified the role of vector and tensor constants of the motion. These have their meaning in a potential such as a spherically symmetric potential for which there is a set of operators satisfying angular momentum commutation relations. Vectors and tensors are defined by their transformation rules in such circumstances, so there is no problem in writing down the commutation rules (either as commutators or as Poisson brackets) which their components must satisfy with respect to the angular momentum components. Angular momentum operators may be written as differential operators acting on a function space, so that there result differential equations which must be satisfied by the components of the putative vector or tensor operator. Their solution admits a slight generalization of the Runge vector of the hydrogen atom, or the tensor operator of the harmonic oscillator, but considerations of single valuedness seem to rule out all such operators with the exception of the ones already known. Bacry *et al.* (149) have investigated most of the possibilities.

## XIV Universal Symmetry Groups

Perhaps one of the most interesting ideas to emerge from the recent activity is the concept of a universal symmetry group, which, since it would be the group  $SU(n)$ , might be thought to underlie some of the success of unitary groups in explaining the elementary particle spectrum. The universal symmetry group has its inception in an alternative approach to the explana-

tion of accidental degeneracy, based more on the harmonic oscillator than on the hydrogen atom. In other words, the hydrogen atom is rather closely associated with the concept of stereographic parameters, both from their occurrence in Fock's transformation which makes the hyperspherical symmetry geometrically evident, and the role of the conformal group as a noninvariance group. Here it might be noted that Lumming and Predazzi (150) have undertaken to extend the class of potentials which might have  $O(4)$  symmetry in terms of the hypersphere and found nonlocal potentials meeting the requirements; and that the monopole problem which has  $O(4)$  symmetry cannot possibly admit a reduction to the hypersphere, since it involves representations of  $O(4)$  which cannot be realized by orbital angular momentum operators. Nor can such a hyperspherical interpretation be given for the "symmetric" Dirac equations with electric or magnetic Coulomb potentials.

Stereographic parameters also enter into the explanation of the accidental degeneracy of the harmonic oscillator, but here the situation is rather different because the stereographic parameters can be recognized as the action-angle variables for the harmonic oscillator with a certain fairly plausible system of coordinates for its phase space (21). Consequently, if the geometric interpretation is slightly more artificial than for the hydrogen atom, it is more closely allied with the precepts of classical mechanics. Since the action-angle variables are involved, it is possible to describe the constants of the motion in a form applicable to any kind of coordinate system in which the Hamiltonian is a function of a certain type of combination of the coordinates and momenta.

This form is actually extremely simple: We define

$$a_k^\pm = \mp i (J_k/2\pi)^{1/2} \exp(\pm 2\pi i w_k),$$

where  $J_k$  is the  $k$ th action variable and  $w_k$  is its conjugate angle, whereupon we find that the Poisson bracket commutation rules

$$\begin{aligned} \{a_i^-, a_j^-\} &= 0, & \{a_i^+, a_j^+\} &= 0, \\ \{a_i^+, a_j^-\} &= 2i \delta_{ij}, \end{aligned}$$

are satisfied; that accordingly, constants of the motion are given by

$$k_{ij} = a_i^+ a_j^-;$$

and that their own mutual commutation rules are simply those for the unitary group  $U(n)$ . If account is taken of the relationship

$$\mathcal{H} = \frac{1}{2} \sum_i a_i^+ a_i^-$$

to extract the trace of this tensor operator, the remaining components will satisfy the commutation rules of  $SU(n)$ .

Very similar conclusions were drawn by Mukunda (151), Fradkin (152), Maiella and Vitali (153), Rosen (154), and perhaps other authors. One can vary the claims as to the generality of the system of  $n$  degrees of freedom for which he can construct an  $SU(n)$  symmetry group. That the theory applies immediately to classically degenerate systems, by which we mean that their Hamiltonian is of the form given above, there is no question. However, it is one of the basic tenets of the Hamilton-Jacobi theory that all systems can be reduced to force-free

motion in some sort of appropriately chosen space. Questions of the topological structure of the space intervene, as well as some as to the unicity of the canonical transformation required, but subject to this restraint, all problems should be reducible first to force-free motion and thence to the harmonic oscillator.

One does not need to go beyond classically degenerate systems, however, to encounter his first difficulties. The Kepler problem in polar coordinates is assuredly a classically degenerate problem, which should yield the symmetry group  $SU(3)$ . Yet, this is the very model of a problem whose hidden symmetry group is  $O(4)$ , and these two groups are not precisely the same, nor is one a subgroup of the other, nor are they isomorphic or homomorphic. The dimensions of their representations are very different.

Dulock (155) found a mapping, neither linear nor a homomorphism, from the one group to the other. The groups can still be somewhat related geometrically, since the tensor constant of the motion of  $SU(3)$  has three eigenvectors. Not surprisingly these turn out to produce the angular momentum, the Runge vector, and a vector determining the line of nodes.

In a sense, Dulock's mapping only compounded the confusion, since the irreducible representations of the two groups are so entirely distinct. Perhaps the confusion is only apparent, however, for recently Ravenhall *et al.* (156) found that the irreducible representations of  $SU(3)$  which occur in the harmonic oscillator could be made to span two irreducible representations of  $O(4)$ , and conversely, a single irreducible representation of  $O(4)$  found in the harmonic oscillator spectrum could be made to span two irreducible representations of  $SU(3)$ . In other words, one can actually realize Dulock's conclusion that  $SU(3)$  might be a symmetry group for the hydrogen atom if he confines himself to states of a definite parity. In any event, Cisneros (25a) has confirmed that this relation between the orthogonal groups and the unitary unimodular groups is a quite general one, and there seems to be some hope that Dulock's mapping can be established generally as well.

The idea that a single uniform construction might suffice to establish a certain type of group, such as the unitary unimodular group for the appropriate number of degrees of freedom, as the hidden symmetry group for all single-particle systems of classical mechanics is an extremely attractive one, and is the substance of the idea that there might be a universal symmetry group. No one has been able to find any flaws with such a concept, at least in its milder manifestations in classically degenerate systems, although some enlightening precautions have been found necessary.

Han and Stehle (157) have shown, for example, that  $SU(2)$  is definitively not the symmetry group of the two-dimensional hydrogen atom, a result which has been confirmed quantum mechanically by Cisneros and McIntosh (158). Here, the existence of  $SU(2)$  can most forcefully be seen in parabolic coordinates, but the two-valuedness of parabolic coordinates means that one is left in the end with only the factor group  $O(3)$ . The discrepancy in polar coordinates arises from other, more fundamental causes.

Stehle and Han (159) have examined the whole question of classical degeneracy from the point of view of the old quantum mechanics, and found that one must temper conclusions concerning the pure unadulterated concept of a classical symmetry group with considerations of the unicity of both the transformation group, and the transformation to canonical coordinates which places it in evidence. Generally speaking, the reason for this is that the phase integrals which make their appearance in the Wilson-Sommerfeld quantization conditions also depend upon the concept of a closed cycle in phase space, a definition of which may be modified by a transcendental mapping under which no integral number of closed circuits will pass into an

integral number of circuits in the new space to allow the preservation of the quantization. They then state a more precise criterion for classical degeneracy.

A better understanding of all the problems involved begins to unfold with a more careful discussion of one of the simplest of all possible systems, the anisotropic harmonic oscillator in two dimensions. The classical symmetry group of this system was already found by Jauch and Hill (17) when the two eigenfrequencies were commensurable, and by Dulock, even when they were incommensurable; Cisneros reevaluated Dulock's derivation and found that the group followed immediately from Dulock's principles, already cited. Jauch and Hill had also already encountered the difficulty that was to prove central to understanding the entire failure of the universal symmetry group in quantum mechanics; namely that when they tried to find the quantum mechanical version of their constants of the motion they found that they did not quite satisfy the proper commutation rules; had they been less cautious, they might have fallen into the same difficulty which has beset the theory of quantum mechanical phase operators (160). Demkov finally found an adequate set of generators for the  $SU(2)$  symmetry group of the harmonic oscillator with 2:1 frequency ratio, and uncovered the interesting fact that there in fact occurred two families of irreducible  $SU(2)$  representations. This was the first break with the folkloric tenet that the symmetry group must be such that each irreducible representation should occur only once.

Cisneros finally unraveled the situation for quite general anisotropic harmonic oscillators when he found that in fact several families of irreducible  $SU(n)$  representations occurred, according to the least common multiple of the eigenfrequencies. The operator which determines the residue class of this least common multiple commutes with all the operators of his von Neumann algebra, and consequently their number determines the multiplicity of the von Neumann algebra, and in consequence, of the unitary modular group which is formed from its operators.

In fact, the degeneracy of the harmonic oscillator is most vividly understood in terms of creation and annihilation operators, which transfer quanta of energy from one coordinate to another. When the oscillator is anisotropic, the quanta are not all of the same size, and then it is necessary to group them in common-sized lots, if possible. For incommensurable frequencies, this is not possible. In fact one can see a certain rudimentary continuity as the frequency ratios are varied. The more incommensurable the frequencies, the greater the multiplicity of occurrence of the representations of the unitary unimodular group. Moreover, lower-dimensional representations will generally (but not always) be of lower energy. Thus, with lesser commensurability, there are more and more one-dimensional representations, and the energy gap to the first doubly degenerate level becomes greater and greater. In such a way one can reconcile the fact that the oscillator with incommensurable frequencies has a unitary unimodular symmetry group and no degeneracies. Although the construction involved is not the only way that the universal symmetry group could be attributed to the anisotropic oscillator, it seems to be the only one consistent with the fact that the quantum mechanical ladder operators do not have roots, and thus if they are employed, it must be by use of their integral powers. Of course, it seems reasonable that they may occur along with rather arbitrary functions of constants of the motion and other Hermitian operators.

The understanding of the anisotropic harmonic oscillator is a rather necessary first step toward understanding the universal symmetry group in general, because a great many classically degenerate systems occur with different natural frequencies for the different angle variables. For instance, if the harmonic oscillator is to be separated in polar coordinates, the action

variables occur in the combination  $(2J_r + J_\theta)$ , with a 2:1 frequency ratio. One now encounters some fairly genuine difficulties on account of the fact that Dulock's formula for the ladder operators may involve functions of non-commuting quantum mechanical operators. Fortunately, in some of the simpler systems which one wishes to study, the angular variable is an arcsine or a variable plus an arcsine, so that a tractable rational expression is available as the starting point for the quantum mechanical transcription. If we can trace the fate of the universal symmetry group in some of those examples where its absence is most glaring, it will not be so greatly missed in places where we might never have previously expected to find it.

Since the prediction that the hydrogen atom separated in polar coordinates should have a unitary unimodular universal symmetry group is the one most outstandingly in contradiction with the results that an orthogonal group is the "true" symmetry group, and since equal frequencies arise from the action-angle variables, that would seem to be the system for which an analysis was most urgently needed. It is found that satisfactory ladder operators exist, which reduce to Dulock's operators in the classical limit, and furthermore, as is typical of the cases which have been studied, the ladder operators reduce to the ones found by Infeld and Hull. In fact, there is only one flaw in the commutation rules satisfied by the ladder operators so obtained; a small flaw, but nonetheless fatal. Classically, since they form a set of canonical coordinates themselves, the ladder operators arising from different action-angle variables ought to commute. In the quantum mechanical case, they do not, when applied to wave functions of certain extreme quantum numbers. For all other wave functions, the vast majority of them, the commutation rules are quite correct.

The mechanism seems to be that the wave functions are expressed in a certain coordinate system, polar for example, where the ladder operators depend upon the (polar) action-angle variables. Consequently, it is found that the radial ladder operators influence only the principal quantum number  $n$ . However, the theta ladder operators influence both the principal number  $n$  and the angular momentum quantum number  $\ell$ . Finally, the phi ladder operators, arising from the phi action and the angle variable (not  $\varphi$ ) conjugate to it, operate on all three:  $n$ ,  $\ell$  and the magnetic quantum number  $m$ .

In addition, the ranges of some of the quantum numbers depend on the values of others; in this example,  $\ell$  runs from 0 to  $n$ , and  $m$  runs from  $-\ell$  to  $\ell$ . The difficulty can be illustrated by the wave function with quantum numbers  $(n, -n + 2)$  in two dimensions. Then

$$\mathcal{A}_\theta^- \mathcal{A}_r^+(n, -n + 2) = c(n, -n), \quad \mathcal{A}_r^+ \mathcal{A}_\theta^-(n, -n + 2) = 0.$$

We have used

$$\mathcal{A}_r^+(n, \ell) = (n + 2, \ell), \quad \mathcal{A}_\theta^-(n, \ell) = (n - 2, \ell - 2),$$

where we take a state to be zero if its indices fall outside the allowed range, and thus the  $r$  and  $\theta$  ladder operators do not commute, as they ought. In this way we are released from the responsibility of finding an  $SU(3)$  symmetry group for the three-dimensional hydrogen atom. It is interesting to note that Dulock's transformation maps the operators which do not satisfy quite the proper commutation rules for  $SU(3)$  into a set which actually do satisfy the rules of  $O(4)$ .

It is profitable to construct some further examples, even though they are somewhat artificial. One can always change the coefficient of  $J_\theta$  in any problem separated in polar coordinates by introducing a centrifugal potential proportional to the square of the angular momentum of

the particle. The force is velocity dependent, but the motion can be understood in terms of precession of the motion without the additional potential. By choosing the potential properly, one can change orbits typical of the harmonic oscillator into orbits typical of the hydrogen atom and conversely, and quantum mechanically the same interchange in transformation properties of the wave functions can be made. A basis may be had for understanding the results of Ravenhall *et al.* as well as the traditional close relationship between the hydrogen atom and harmonic oscillator. For our present purposes it is sufficient to note that there are certain frequency ratios ( $J_r + 3J_\theta$ , for example) which lead to degeneracies which could not possibly arise from a Lie group, but nevertheless correspond to closed, bounded orbits. It is just such an impossibility, in the simplest of all possible contexts, which strikes the death blow to the concept of a universal symmetry group, and recommends that we base our thinking on ladder operators rather than symmetry groups.

## XV Summary

In summary, although we may suspect that the last word has still not been said regarding symmetry and degeneracy in single-particle mechanics, we may still feel a satisfaction that some of its aspects at least are now understood. Although it has been primarily a quantum mechanical phenomenon, since degeneracy makes itself most visible in the multiplicity of degenerate energy levels, it turns out that its understanding is not uninteresting for classical mechanics either, one of the more noteworthy by-products of the understanding of the quantum mechanical realm having been the discovery of  $SU(n)$  as a universal symmetry group for classical mechanical systems. Needless to say, it is a disappointment that one could not have retained  $SU(n)$  as a quantum mechanical symmetry group as well, for it might then have been found to have some relation to the currently fashionable classification schemes for elementary particles. Even so it may still retain some utility in the limit of large quantum numbers, for which the effects of quantization wreak lesser havoc on the classical concepts.

The development of the theory of symmetry reflects in an interesting way the development of quantum mechanics and even present-day physics itself, presenting in a subtle way the suspicion that we do not really understand the workings of any physical process until we understand fully its symmetry properties. The history of the Dirac equation provides a nice illustration of this point. It has been a puzzle ever since its creation in 1928, although it immediately accounted for the electron spin and the experimental fine structure of the hydrogen atom. These were great successes, because the electron spin had previously been a purely *ad hoc* assumption, and the failure of the Klein-Gordon equation to give the hydrogen fine structure had left it in disrepute. However, the discovery of *Zitterbewegung* left a distinctly uneasy feeling about the mechanical interpretation of the movement of an electron, and the negative energy states which occurred in the solution required a definitive reformulation of quantum mechanical thinking, first with the introduction of the hypothesis of the electron sea and later with second quantization and the use of field theory. It was only after two decades, in 1950, that the Foldy-Wouthuysen transformation clarified the separation of positive and negative energy states, and set the *Zitterbewegung* in its proper perspective. It was at this same late date that the constant of the motion responsible for the residual twofold accidental degeneracy in the relativistic hydrogen atom was found by Johnson and Lippman.

Even then, it remained for the parity nonconservation experiments to show how incomplete

the examination of the possible reflective symmetries of the Dirac equation had been, and another full decade before Biedenharn began to tamper with the Dirac Hamiltonian to produce a system with the degeneracy of the nonrelativistic hydrogen atom, and thus to begin to clarify the entanglement of relativistic effects with the spin-dependent, or more properly the multicomponent, aspects of the Dirac equation.

In the meantime, the Klein-Gordon equation has been rehabilitated and seen to apply to pi-mesonic atoms, relativistic wave equations have been written for systems with other intrinsic spins, and even the Dirac equation reformulated in alternative ways, including the two-component, second-order form introduced by Feynman and Gell-Mann.

To what should one attribute the degeneracy which occurs in many systems? Hidden symmetry is an attractive explanation, especially since the most generally known systems have had a very elegant interpretation in terms of hidden symmetry of one sort or another. However, it might seem that the existence of ladder operators and the separability of the equations of motion might be a sounder and more extensive basis from which to attempt the investigation of degeneracy. From the work of Infeld and Hull we know that ladder operators can be constructed for the most general sorts of second-order linear differential equations, of the type which habitually arises from quantum mechanical problems. Thus, separability seems to be the prevailing requirement, and ladder operators may be formed for separable systems even when there is no degeneracy at all. Degeneracy is then to be considered an exceptional circumstance depending upon the relative size of the steps taken by the various ladder operators. Moreover, even when there is degeneracy present, we have seen that it may not necessarily lead to the existence of either a small Lie group or to particularly interpretable transformations of phase space.

The foregoing remarks do not detract in any way from the beauty or elegance of the hidden symmetry concept in those situations where it applies, but they do limit the generality of such a concept as an interpretation of accidental degeneracy in every situation. In fact it is by no means clear at the present moment whether or not the classification of elementary particles will one day be fitted into a scheme resembling the harmonic oscillator or the bound states of the Kepler problem, wherein there will be not only symmetry operators but ladder operators running between different energy states, in such a way that the entire energy spectrum may be interrelated. Should such a systematic structure be found, it will no doubt rank with Mendeleev's table of the chemical elements or the scheme of nuclear magic numbers as a major triumph in our attempts to organize natural phenomena.

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