Quantization as an Eigenvalue Problem*

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* *Group Theory and its Applications* (E.M. Loebl, ed.), Academic Press, New York, 1975. pp 333-368.

1 Quantization

Almost half a century, and with it nearly two entire generations of physicists, has now elapsed since those years in the middle twenties during which quantum mechanics finally crystallized into its presently accepted and universally used form The most fundamental and productive version of quantum mechanics has always been the one introduced by Erwin Schrödinger [1] in the first months of 1926. It was slightly preceded by Heisenberg's matrix mechanics, a discipline which was quickly refined and promptly presented in Born and Jordan's book, *Elementare Quantenmechanik* [2]. Not long thereafter both Dirac [3] and von Neumann [4] produced their two quite unlike operator versions, essentially completing the conceptual foundations of quantum mechanics

The symbolic and operational techniques have been indispensable in providing a vocabulary for the teaching, discussion, and application of quantum mechanics. Nevertheless when the moment arrives that matrix elements have to be calculated and results obtained, it is the Schrödinger equation which is eventually introduced and has to be solved

We must recall that the substance of Schrödinger's papers, indeed their very title, was the assertion that quantization was an eigenvalue problem. By the selection of a suitable diflerential equation and the imposition of satisfactory boundary conditions we were inexorably led to the quantization which was at once the basis and the most singular and inexplicable feature of Bohr's older quantum mechanics. It is especially to be noted that the term "eigenvalue problem" refers to the acquisition of suitable solutions of the boundary value problem of the differential equation, and not to the mere diagonalizalion of a matrix, as the phrase is so often understood nowadays.

However, the specification of the boundary conditions in a way which would be adequate for axiomatic considerations was a concern of some delicacy. Differing viewpoints emerged almost at once, and have persisted in one form or another up to the present day. Schrödinger himself simply imposed the requirements of continuity, single-valuedness, and finiteness. He carefully left the function which actually solved his differential equation devoid of meaning, in spite of an avowed desire to interpret it as a charge density. Eventually, and primarily through the efforts of Max Born, the square of the wave function came to have a probabilistic interpretation, whose natural aftermath was the use of quadratic integrability as a boundary condition.

Unfortunately the requirement of square integrability is not always decisive. There are several instances, one of the most notable of which arises from the ground state of the hydrogen atom, in which all the solutions of the wave equation are found to be square integrable. For s states in the radial equation of the hydrogen atom, there are always two linearly independent solutions, square integrable at the origin. Strictly speaking, we mean that they are integrable in any finite left-hand interval which includes the origin, which is a singular point in the radial wave equation. This means that at whatever energy there can always be found a linear combination which is also integrable in the outward direction, to whatever distance. Thus, according to a criterion of square integrability, there would be no quantization, which is contrary to

observation. In actuality the quantizing principle which is applied is to demand that the wave function be finite at the origin.

There is also a considerable literature devoted to the requirements which angular momentum wave functions ought to satisfy. Again finiteness is the quantizing principle which is used in practice, although periodicity suffices for some of the angular coordinates. Here too, it is found that all the solutions would be square integrable, although sometimes some use can be made of the integrability of the derivative of the wave function, or that the unwanted solutions imply unpalatable currents.

Finiteness at the boundary points does not serve as a universally applicable requirement either, as it is powerless to decide the quantization of some of the levels in the Dirac equation for the hydrogen atom.

Continuum wave functions present a normalization problem of a somewhat different nature. Although it is hardly possible to give a probabilistic interpretation to a wave function which extends over the whole of infinite space with a nearly constant amplitude, it is entirely natural either to speak of relative probabilities, or to work with current densities. The characteristic aspect of continuum wave functions is that they are oscillatory rather than exponential. Consequently their normalization integral grows linearly with the volume over which the wave function extends so that it is sensible to resort to the fiction that their orthonormalily is expressed by a Dirac delta function.

As long as our entire interest lies with bound-state problems, there do not arise too many difficulties about the use of square integrability as a boundary condition, nor is there much opportunity for error in manipulating all operators as though they were finite matrices. Nor is there even much difficulty when operators are defined in a finite closed space, such as the configuration spaces of the quantum mechanical tops or rotors. The exceptions which occur have to do with potentials which are unbounded below, especially with some of the more strongly singular potentials.

Investigators who have had the most practical encounters with continuum wave functions, such as the ones which arise in solid state theory or in scattering theory, have always been able to treat them in a very pragmatic manner, which consists mostly in separating bounded solutions from unbounded ones, and among the bounded solutions classifying them as to their direction of propagation The first initiatives were taken by Born, who was particularly anxious to understand the quantum aspects of scattenng theory. Under his influence, Oppenheimer [5] made some of the first extensions of the Schrödinger equation to aperiodic systems, such as arose in the theory of collisions or passage through barriers.

In one way or another it has usually been possible to set up boundary conditions which would produce a satisfactory resolution to the quantization of any system of practical interest. Strongly singular potentials constitute practically the only significant exception. Inasmuch as there are no physical situations in which they occur in their mathematically pure form, there has never been any experimental evidence which would clearly confirm or contradict speculations as to whether or not quantization would occur, or how to achieve it if it did.

Historically, if there had not always existed quantizing principles sufficient for

the task at hand, there would certainly have been a concerted effort to resolve the uncertainties which might have existed. Yet it is fair to say that there has never been a single, generally understood, and consistently applied criterion, leaving the procedure to he followed in an unfamiliar case quite cloudy.

We might say that square integrability sufficed for bound-state problems whose potential was bounded below, that an occasional finiteness argument was required for moderately singular potentials, that strongly singular potentials never became an issue, and that continuum wave functions never needed quantizing. Rather, the difficulty with continuum wave functions consisted in the incorporation of their mathematical properties into a theory reminiscent of the theory of finite matrices, which the use of the delta function accomplished to most people's satisfaction.

It would seem that there has been another historical process at work, pertaining to the mathematical sophistication of the physicists and others who needed to use quantum mechanics, and perhaps also to the sophistication of the mathematics with which quantum mechanics itself was phrased. Schrödinger was able to formulate quantization as an eigenvalue problem, precisely because he was familiar with the development which Hilbert had given to eigenvalue problems, and which had been worked out quite precisely for second-order differential equations by Hermann Weyl. The only complication which continuum wave functions caused in an eigenfunction expansion was the necessity to employ a Stieltjes integral in place of a sum on many occasions. Von Neumann met the same difficulty in formulating his theory of operators on Hilbert space, which he likewise resolved wilh a Slieltjes integral over projection operators. Unfortunately use of the Stieltjes integral never became a standard part of the "mathematical methods of physics."

The reason was most probably the fact that the "eigendifferentials" which occurred in the integral were somewhat hazy concepts, and did not approach a limit having a clearly defined conceptual significance, which was natural. Otherwise it would never have been necessary to resort to the Stieltjes, rather than a Riemannn, integral in the first place. Since the result was to introduce a language which appeared to physicists to involve some rather elaborate circumlocutions which they found bothersome, the mathematical presentations, although quite accurate, never enjoyed much popularity.

2 Operators on Hilbert Space

Kemble's Fundamental Principles of Quantum Mechanics [6], one of the first and certainly the most scholarly of the early books on quantum mechanics to be published in the United States, despaired of Weyl's theory, commenting "The problem has been treated bv Weyl in a basic paper which unfortunately involves an elaborate mathematical technique and makes difficult reading for the non-specialist." By and large the general tendency has been to use Dirac's symbolism, and to treat all wave functions as though they were normalizable. even when such was not the case.

Schwartz's theory of distributions nowadays provides the opportunity to legitimize most of this work from the rigorous mathematical point of view, although it does not

seem to have contributed much additional physical insight.

The use of a theory operators on Hilbert space has sometimes engendered the feeling that the problem of specifying boundary conditions has been sidestepped. In reality it is only recast in a different form, but by a mechanism - the specification of a domain - which merits attention.

A Hilbert space theory of differential operators is complicated by the fact that differentiability and square integrability are really two quite different concepts. Integrability is a global characteristic whereas differentiability is a local property. Thus Hilbert space includes many functions which have mathematically unpleasant aspects, such as lacking derivatives or being discontinuous. Yet at the same time it lacks numerous functions considered to be important, such as the powers or the complex exponentials.

As a result we frequently find that the quantum mechanical operators can be applied in a meaningful way to functions which do not belong to Hilbert space, whereas at other times it happens that they cannot be applied to some of the legitimate members of Hilbert space.

The situation is a fundamental one, and the result is that for every operator on a Hilbert space there must he specified its "domain," which is to say. the collection of functions to which we propose to apply it. It is through the definition of the domain that the boundary conditions of differential operators frequently enter, often without there being overt recognition of the fact. The selection of a domain for an operator is of the utmost importance; if the domain is too small, the operator may not be adequately defined, but if an attempt is made to make the domain too large, the operator may simply be impossible to define. Moreover, the Hermiticity of an operator may depend on the proper selection of its domain. A final precaution, one which is too often overlooked, is the verification that two or more operators, when they are employed in a common calculation, either have a common domain or the calculation purports only to refer to the domain which they share in common. Nevertheless, once there is an adequate realizalion of the limitations of Hilbert space theory, there is a vast reservoir of rigorously demonstrated mathematical results waiting to assist calculations and the endeavor to solve Schrödinger's equation. Hilbert space theory and differential equation theory can be used in harmony, without the necessity to give up such things as continuum wave functions because of their nonnormalizability.

At the beginning of this century the theory of differential operators was already rather extensively developed, especially with regard to the classification of the singularities which could occur in the solulions as a consequence of singularities in the coefficients, or of the infinitude of the interval of integration. But we might say that the theory of differential operators commenced with Hermann Weyl's investigation of the relationship between square integrability of the solutions and the boundary conditions to which the equation was subject. These results appeared in the *Mathematische Annalen* of 1910 [7].

Although Weyl's article was frequently cited in succeeding years, it was limited to ordinary second-order singular differential equations, and did not seem to motivate any great amount of further study for some 30 years. Then, E. C. Titchmarsh began a

systematic analysis of the properties of eigenfunction expansions according to the solutions of differential equations, which he published in numerous papers in the British mathematical journals. Eventually these papers formed the skeleton of his two-volume treatise [8] on eigenfunction expansions which was published after the war. The first time that Weyl's theory was available in a popular English language textbook seems to have been with the publication of Coddington and Levinson's authoritative *Theory of Ordinary Differential Equations* [9] in 1955.

At present, with the appearance of Dunford and Schwartz's massive three-volume *Linear Operators* [10], whose bibliography alone exceeds 100 pages containing nearly 2000 references, we have a completely overwhelming, albeit encyclopedic compendium of the whole subject. Nor should it be overlooked that there is also a considerable Russian literature, whose growth commenced mainly in the 1940's.

A comprehensive and straightforward theory of partial differential equations is still hard to come by, in spite of the importance of these equations and the vast amount of theoretical and computational effort which has been expended on them over the years. Fortunately there is one exception, which practically speaking is a very important one, whereby it is possible to refer the analysis of separable partial differential equations to systems of ordinary differential equations, which are much more tractable.

The bulk of the partial differential equations which physicists, chemists, or engineers solve are separable. Other kinds are very much more difficult to resolve, and so do not receive so much attention. Yet, given the spherical symmetry inherent in many problems of interest, and given the applicability of the Hartree-Fock equations which originate in an approximation based on separability, it would suffice for the understanding of a sizable class of problems of practical importance to arrive at a good understanding of ordinary differential equations. Separable problems, at least, can then be resolved by combining all their constituents, once each has been worked out individually.

In a sense, the point of view presented here has already been worked out extensively during the past two decades in the guise of Regge pole theory, dispersion relations, analytic S-matrix theory, and related topics. Two characteristics of that work may explain the reason it is not more widely known. It was carried out mainly in those branches of high-energy physics which were primarily concerned with scattering theory, and for which bound states were of secondary importance, even somewhat undesirable. Additionally, the properties of angular momentum were inextricably mixed with the energy dependence of the wave functions. Indeed. Regge [11] began his program to apply the Watson transform to quantum mechanics knowing how successfully it had been used by Sommerfeld to sum the partial waves arising in the theory of the propagation of radio waves over a spherical earth. As the presence of angular momentum is the only possible consequence of separation in spherical coordinates, we cannot complain.

Returning to the contention that the architects of quantum mechanics must have been content with the sufficiency of their quantizing principles, we are substantially left with an evaluation of von Neumann's *Mathematical Foundations of Quantum Mechanics* [4]. There differential equations have been replaced by operators on Hilbert space, their boundary conditions subsumed in the selection of a domain. Quanitzation

transpires in the Hermiticity of the Hamiltoman: to have this property the Hamiltonian operator must certainly be "hypermaximal," which can become an issue for the singular potentials. Their naive Hamiltonian is not hypermaximal. To make it so requires a "self-adjoint extension" which amounts to restricting the domain. This implies an additional boundary condition, the same one which arises in the "limit circle" alternative for Weyl's theory of differential operators. Whether the extension has a physical significance does not concern the mathematical theory, so it is said that we should have no trouble with the singular potentials.

What about the continuum? We learn that the spectrum of an operator $\mathcal{H}$ is to be defined by the nonexistence of the resolvent, $(\mathcal{H} - \lambda\mathcal{I})^{-1}$. For finite matrices the inverse may simply not exist, the responsible vector is annihilated by $(\mathcal{H} - \lambda\mathcal{I})$ and is thus an eigenvector. For operators a second possibility is that the resolvent is not bounded. The former situation defines the discrete spectrum – the only possibility for finite matrices – but the second leads to the continuous spectrum. The would-be eigenvectors are afflicted with an infinite norm; they may well enough exist, but they do not belong to Hilbert space. Infinity, in Hilbert space, may contain some very respectable functions. Instead we must deal with approximations, which are not quite eigenvectors, but which do belong to Hilbert space. These are Weyl's eigendifferentials. So much for the continuum; our discomfiture lies in being deprived of those nonnormalizable eigenvectors.

The demand that the Hamiltonian be Hermitean is apparently an adequate quantizing principle; at any rate it was sufficiently salisfying in the historical development of quantum mechanics that the question lay dormant thereafter. However, it is to be seen that the emphasis had shifted subtly from the solution of a differential equation to an operator calculus. If the differential equation is fundamental, we at least have to know how to relate its solutions to physical processes, which to date has always been through a statistical interpretation of the wave function. If we are to use an operator calculus, we had better know how to choose the operator corresponding to a given physical process.

There seem to be opposites involved here: take the differential operator and make the best of its solutions, or take a theory of probabilities and try to find the best operator to fit the circumstances. Maybe there is a middle ground. Perhaps both of these extremes tend to impose constraints on a problem which has yet to be thought through in its entirety.

In either event, it is clear that the theory of operators has not yet been understood completely, and this in spite of the prodigious size of the more ambitious treatises. Nor has the theory of differential equations been explored to its conclusions. Nor is the popular understanding of either theme commensurable with then present states of development. With these thoughts in mind, it could be interesting to explore the relationship between a differential equation and its boundary conditions.

Operator theory would like to delegate the boundary conditions to the axiomatic preliminaries, which is to say that in any given instance they enter into the formalities wherein it is verified that the axioms are satisfied, so that we can proceed with the important business of mathematical deductions and proving theorems. Differential

equation theory tends to be somewhat preoccupied with establishing the existence and uniqueness of solutions, the conditions which favor the establishment of boundary conditions, and similar matters.

3 Differential Equation Theory

However, the real role of a differential equation lies in relating conditions in one region to those in another, through a recursive process which allows us to progressively work out the solution fiom one place to another, a little bit at a time. The framework is prescribed by the differential equation, but the information which is to be relayed from one place to another is contained in the boundary conditions. We need not grieve if the system is capable of sending more information than we shall ever attempt, which is another way of interpreting the fact that the differential operator may have eigenfunctions which do not belong to Hilbert space while we want to confine ourselves to square integrable functions. The other anomaly which may arise is that the system is incapable of transmitting cerlain information, or of transmitting it in certain ways. This would seem to be the failure which occurs for the strongly singular potentials.

Probably the most fundamental aspect of the whole theory of differential equations is the existence of a Green's formula. These are formulas which relate integrals invoking the solutions of a differential equation to its boundary values. The name is chosen because of the analogy to relations occurring in the early theory of electricity by which numerous volume integrals could be transformed into surface integrals These were introduced by Green in a pamphlet published in I828 [12].

From a mathematical point of view such integrals correspond to bilinear or quadratic forms. A Green's formula permits them to be expressed in terms of their boundary values, through a process akin to integration by parts. In terms of vector space concepts, the result is a mapping from a large-dimensional space which would be comprised of all possible functions, of which there is a subspace which is highly constrained consisting; of those functions which actually solve the differential equation. The mapping is from this rather small-dimensional subspace of possible solutions, which is embedded in a very much larger space, to the space of boundary values. The boundary values are in one-to-one correspondence with the solutions and are free from any constraints.

Bilinear forms and norms are very intimately related: in a Hilbert space they determine one another. It is through the mapping of a norm or the bilinear forms in function space to their counterparts in the boundary value space that the theory or operators on Hilbert space becomes involved in the solutions of differential equations. The crucial point to be observed is that the theory only relates the norms to one another, without in any way implying that the solutions of the differential equations have to belong to the Hilbert space. Misunderstanding of this point has been principally responsible for the conceptual difficulties surrounding continuum wave functions.

Bilinear forms are mapped from the solution space to the boundary value space in a rather curious way. Positive-definite bilinear forms become symplectic bilinear forms in the boundary value space. Because of its anti-Hermitian character a symplectic

form vanishes identically for equal but purely real arguments. Should an equality between symplectic forms involve such arguments, it would he somewhat vacuous.

Two avenues for obtaining information are then open: one is to take limits, the other is to use complex solutions to the ditferential equation. The former approach leads to the classical Christoffel-Darboux formulas and a number of useful relationships involving derivatives of solutions. The complex approach allows us to use the full apparatus of complex variable theory, in particular the possibility of analytic continuation with respect to the eigenvalue parameter. It is found that the resulting class of functions is sufficiently interesting to warrant that line of approach.

Oddly enough, when we come to regard a differential equation as serving only to define a mapping from the solution space to the boundary value space, it is possible to avoid an excessive preoccupation with the actual boundary values themselves. Such a maneuver docs not avoid the formulation of boundary conditions, but it sets them aside into another category, and at the same time permits approximations to be made. This is yet another way to work with wave packets, which approximately solve the differential equation, or which approximately meet the boundary conditions, as most suits the convenience of the moment.

Among the functions which can be obtained with the help of a Green's formula, by far the most important of them all is the spectral density function. Such a function has been familiar to electrical engineers as the complex impedance of a continuous line, and to physicists as the Jost function or as the S-matrix. Strictly speaking the crucial function is the Titchmarsh-Weyl m function, whose imaginary part over the real axis is the spectral density. On account of its being the imaginary part of the boundary value of an analytic function, possibilities exist for its analytic continuation, to write dispersion relations for it, and for activities of a related nature. Such relations have been extensively studied by theoretical physicists in other contexts.

It is worth examining the derivation of the spectral density wilh some care, considering its importance for a general theory.

To begin with, the one-dimensional, time-independent Schrödinger equation can be written in the standard self-adjoint form

$$\left\{-\frac{d}{dx}p(x)\frac{d}{dx}+q(x)\right\}\psi(x) \quad = \quad \lambda\psi(x)$$

Here $\psi(x)$ is the wave function, $q(x)$ is the potential energy, while λ is the energy, appearing in the equation in the role of an eigenvalue parameter. The weight function $p(x)$, assumed always to be strictly positive, may arise sometimes from the separation of variables in non-Cartesian coordinate systems. Units of distance and energy have been so chosen that the purely physical constants do not make an appearance explicitly anywhere in the equation.

It is convenient to introduce the operator symbolism

$$\mathcal{L}[\psi] \quad = \quad \lambda\psi$$

which can be used to summarize the differential equation which we have written, as well as eventually others, such as the one-dimensional Dirac equation.

Green's formula can be obtained from an integration by parts: it states that

$$\int_a^b \{\varphi^* \mathcal{L}[\psi] - \mathcal{L}[\varphi]^* \psi\} dx \quad = \quad [\varphi, \psi]|_a^b.$$

The bracket, which we have indicated on the right-hand side of the equation, is defined by

$$[\varphi, \psi](x) \quad = \quad -p(x)\{\varphi^*(x)\psi'(x) - \varphi'^*(x)\psi(x)\}.$$

It is somewhat more suggestive to write a self-adjoint second-order differential equation as a pair of coupled first-order equations, preferably in matrix form. We could then write

$$\frac{d}{dx}\begin{pmatrix} \psi \\ p\psi' \end{pmatrix} \quad = \quad \begin{pmatrix} 0 & 1/p \\ q-\lambda & 0 \end{pmatrix}\begin{pmatrix} \psi \\ p\psi' \end{pmatrix}.$$

In turn we are permitted to write the bracket in the form

$$[\varphi, \psi] \quad = \quad \begin{pmatrix} \varphi^* & \varphi'^* \end{pmatrix}\begin{pmatrix} 0 & -p \\ p & 0 \end{pmatrix}\begin{pmatrix} \psi \\ \psi' \end{pmatrix}.$$

Given such a representation, it is quite clear that the bracket is a bilinear form defined by an antisymmetric metric matrix. Let us adopt a quaternionic notation for the $2 \cdot 2$ Pauli matrices:

$$\mathbf{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{1}^t \qquad \mathbf{i} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \mathbf{i}^t$$
$$\mathbf{j} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = -\mathbf{j}^t \qquad \mathbf{k} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{k}^t$$

By doing so we can incorporate the one-dimensional Dirac equation into this same scheme of notation. According to Coulter and Adler [13] we might write such an equation in the form

$$\frac{d\psi}{dx} \quad = \quad (E\mathbf{j} - V\mathbf{i} + m_o\mathbf{i})\psi$$

with energy E, potential energy V, and rest mass m_0. ψ is now a two-component vector.

Define the operator $\mathcal{L}$ by

$$\mathcal{L}\psi \quad = \quad \left(-\mathbf{j}\frac{d}{dx} + V\mathbf{1} - m_0\mathbf{k}\right)\psi$$

Supposing that the inner product in the solution space for the Dirac equation involves the sum of the absolute squares of both components, we can deduce a Green's formula

$$\int_a^b \{\varphi\mathcal{L}\psi - (\mathcal{L}\varphi)^t\psi\} dx \quad = \quad -\varphi^t\mathbf{j}\psi|_a^b.$$

Again, the presence of the antisymmetric metric matrix assures us that the boundary values will follow a symplectic geometry.

The Dirac equation for three-dimensional, spherically symmetric potentials can be cast into a rather similar form, once the angular variables have been separated. The radial equation which remains consists of the same pair of coupled first-order equations which arises for the one-dimensional Dirac equation.

Regardless of the context, the derivation of a Green's formula, which primarily involves inventing an appropriate anti-Hermitian form for the boundary space, is a crucial step. Once such a formula is available, the remaining steps in the derivation which we shall outline forthwith remain virtually unchanged, whatever the differential equation which is under discussion. It is fortunate that it is possible to discover an adequate formula in the widest variety of situations. Roos and Sangren [14] have shown how the brackets may be obtained for the pair of equations corresponding either to the one-dimensional Dirac equation or the radial part of the three-dimensional Dirac equation. Their procedure is much as we have discussed it above. Kodaira [15] has obtained a bracket for a differential operator of arbitrary even order while Everitt [16] has studied the particular case of fourth-order operators quite exhaustively. Similar constructions are possible for systems of differential operators, as well as for partial differential operators.

Green's formula is particularly effective when it is applied to eigenfunctions of the differential operator from which it was derived. Supposing that

$$\mathcal{L}[\varphi] \quad = \quad \lambda\varphi, \qquad \mathcal{L}[\psi] \quad = \quad \mu\psi,$$

we obtain

$$(\mu - \lambda^*) \int_a^b \varphi^* \psi dx \quad = \quad [\varphi, \psi](b) - [\varphi, \psi](a)$$

Using the traditional parentheses to denote an inner product in the solution space, this equation finally relates the two bilinear forms: the parentheses in the solution space and the brackets in the boundary value space.

A particularly important case results when $\lambda^* = \mu$, which will occur whenever both φ and ψ belong to the same eigenvalue, tempting us to apply Green's formula to φ^* and ψ. In such a case. the left-hand side of the equation uses the real inner product in the solution space, which does not matter because it has a zero multiplier of the form $\lambda - \lambda$.

If we define

$$W[\varphi, \psi] \quad = \quad [\varphi^*, \psi],$$

we obtain, for functions belonging to the same eigenvalue of $\mathcal{L}$,

$$W[\varphi, \psi](a) \quad = \quad W[\varphi, \psi](b),$$

4 Symplectic Boundary Form

The real version of the bracket belonging to a second-order differential operator is the Wronskian of two solutions. For higher order operators it is a bilinear version of the corresponding Wronskian, which itself is multilinear. The most interesting property of the Wronskian of a self-adjoint operator is its constancy, which is a fundamental property shared by the real bracket, whatever the order of the differential operator. This result is so familiar that we might pass right over it without noticing that it is really an invariance principle, which asserts that the real bracket is a bilinear form which is invariant under the choice of a boundary point at which to evaluate it, so long as its arguments are two solutions belonging to the same value of the eigenvalue parameter.

Here, as elsewhere, we find that we must on occasion use both the complex as well as the real variant of the bracket, so that it is not possible merely to define the one and ignore the other. Indeed, considerable confusion may be avoided by expending the effort required to set down the properties of each one of them separately, to the extent that it is possible to think readily of them independently and iis as having their own individual characteristics.

Calculation of the complex bracket

$$(\varphi, \psi) \quad = \quad \frac{1}{\lambda - \lambda^*} \{ [\varphi, \psi](b) - [\varphi, \psi](a) \}$$

furnishes the desired mapping between the Hermitian inner product of the solution space and the anti-Hermitian bracket in the boundary value space, once again presuming that both of its arguments belong to the same eigenvalue. The practical consequence of this relationship is that the natural adjunct of a Hermitian geometry in the solution space is a symplectic geometry in the boundary value space.

Symplectic geometry is rather similar to the orthogonal geometry of Euclidean space or the Hermitian geometry of complex space, with the exception of the antisymmetry of its metric matrix and the consequent self-orthogonality of all vectors. In place of an orthonormal basis we must construct a canonical basis, whose idiosyncracies are familiar to all persons who have worked with Poisson brackets and canonical coordinates in classical mechanics. When this contrast is borne in mind most activities can be carried out in their accustomed manner. These include use of the Gram-Schmidt process to construct a canonical basis, use of the Gram matrix or the Gram determinant to ascertain linear dependence, or construction of conjugates to aid in the isolation of components of a vector.

Characteristically, canonical coordinates partition space into two parts, in a fashion very reminiscent of the coordinates and momenta into which phase space is divided. For boundary value problems this splitting is particularly compatible with the most common specifications of separated Sturm-Liouville boundary conditions, wherein half of them are imposed at the left-hand boundary as initial conditions and the remaining half at the rightmost boundary point as terminal conditions.

Many occasions arise for comparing constraints imposed on a function at one point to those which have been imposed at some other point. The strongest motivation for

these mutual comparisons is the circumstance that the initial-value problem is always uniquely solvable, providing the best conditions of reference for the solutions upon which other kinds of restrictions have been imposed. Two rather complementary procedures can be implemented to achieve such a comparison. One is to reduce a restriction at a given point to an equivalent restriction at the initial point, by solving the differential equation backwards and comparing constraints. The other is to extend a solution of the initial-value problem to the point of comparison. Comparisons are most satisfactorily made by selecting a set of standard initial conditions — preferably a canonical set — whose solutions can then be compared with the solution or with the intended constraints at any other point.

Invariance of the bracket means that the comparison can he obtained by doing nothing more than calculating the bracket between constraints at any given point and the values of the standard solution at the same point. This technique was used quite effectively by Kodaira [15] in forming a general theory of even-order differential operators.

The complex bracket is not positive definite, so that it has a nontrivial null space consisting of those boundary values f which satisfy the requirement

$$[f, f] \;=\; 0$$

Recalling that a Minkowski space is one in which there is a symmetric but not definite metric, we see the null space of an antisymmetric metric as the analog of the light cone of a Minkowski space.

A null space is a homogeneous space, meaning that all the nonzero multiples of an element either belong to the space or not, but simultaneously. The sum of two null vectors is not necessarily null, so that the null space is not necessarily a linear space. For the characterization of the null space it is convenient to introduce a basis in the boundary value space; preferably this basis should consist of the local values of boundary functions. These in turn are best defined by a canonical set of initial conditions.

With respect to a basis an algebraic expression of the second degree is obtained for the coefficients of the null vectors; for second-order differential operators there results a circle in the complex plane. Higher order operators lead to higher dimensional ellipsoids which of course are more difficult to represent graphically.

To obtain this circle we introduce the definition

$$f \;\;=\;\; \varphi + m\psi$$

which exploits the homogeneity of the null space to employ the single coefficient m, which will depend analytically on the eigenvalue λ . The basis functions φ and ψ are required to meet some suitable initial conditions. As already noted, initial conditions are most conveniently expressed in terms of the real bracket and a canonical set of initial values. In the general case there would be a set of vectors $\{\alpha_i, \beta_i\}$ for which we would require

$$W[\varphi, \alpha_i] = 0, \qquad W[\varphi, \beta_i] = 0$$

In turn, the assertion that they form a canonical basis consists in requiring that they fulfill the conditions

$$[\alpha_i, \alpha_j] = 0, \quad [\beta_i, \beta_j] = 0, \quad [\alpha_i, \beta_j] = \delta_{ij}$$

In the special second-order case, the requirement that

$$W[\psi, g] \quad = \quad 0$$

is equivalent to stipulating that g be a multiple of ψ.

Written out in terms of the basis, the null space acquires the form

$$[\varphi + m\psi, \varphi + m\psi] \quad = \quad 0$$

Expansion and some algebraic rearrangement yields

$$\left\{ m + \frac{[\varphi, \psi]}{[\psi, \psi]} \right\} \left\{ m + \frac{[\varphi, \psi]}{[\psi, \psi]} \right\}^* \quad = \quad \frac{W[\varphi, \psi]}{[\psi, \psi][\psi, \psi]^*}.$$

We readily enough recognize the equation of a circle, C_b, whose center is

$$z_b \quad = \quad -\frac{[\varphi, \psi]}{[\psi, \psi]}$$

and whose radius is

$$r_b \quad = \quad \frac{1}{\mid [\psi, \psi] \mid},$$

supposing that initial conditions have been chosen which will make the constant Wronskian in the numerator equal to one.

The somewhat curious result of all this is that the vital statistics of the null surface — for second-order operators, the circle C_b in the complex plane — depend on the integrability properties of the basic solutions of the differential equation $\mathcal{L}[\psi] = \lambda\psi$. Integrability enters through the intermediary of Green's formula, this time applied in the reverse direction to convert the brackets into parentheses

There are three noteworthy points

(1) Any point on the surface of C_b produces a function f whose norm depends only on the initial conditions at a. Therefore, $\parallel f \parallel$ must remain bounded as $b \to \infty$, as long as $m \in C_b$,

(2) For $b_2 > b_1$, $r_{b_2} \leq r_{b_1}$, thus as $b \to \infty$ the radius of C_b decreases monotonically Two cases are of interest (i) $r_b \to 0$ and (ii) $r_b \to \varepsilon > 0$. In case (i), $[\psi, \psi]$ diverges, and with it (ψ, ψ) This is the case which Weyl called the *limit point* case, because the circle C_b must converge to a point In case (ii), $[\psi, \psi]$ is bounded by $1/\varepsilon$. By contrast this is called the *limit circle* case,

(3) Not only is the radius of the circle C_b a monotonic function of b, but the circles themselves each contain all their successors for increasing b, as can be shown by more carefully examining the inequality defining the interior of the circle.

The null surface therefore carries significant information about the square integrability properties of the various solutions of the differential equation For a second-order differential operator it can he inferred, according to the two cases of limit point or limit circle:

Limit Point. From initial conditions specified by a single bracket, in the form $[f, \psi] = 1$, there is always one square integrable solution as $b \to \infty$, namely

$$f \quad = \quad \varphi + m_\infty \psi$$

Any other solution not proportional to this one diverges, in particular, ψ itself is never square integrable over the infinite range.

Limit Circle. Even in the limit as $b \to \infty$ all solutions are square integrable.

Unfortunately we still lack the information necessary for quantum mechanical problems, because the eigenvalue is necessarily complex, forcing us to seek limiting values of m as λ approaches the real axis. Furthermore, in addition to hunting limiting values for m, we still have to investigate the limiting behavior of eigenfunction expansions.

The way in which a connection may be established between eigenfunction expansions in a finite interval and in an infinite interval is to use the theory of Sturm-Liouville systems. For any finite interval it is possible to find a complete orthonormal basis of functions satisfying whatever consistent homogeneous boundary conditions that we wish to impose at the two endpoints. Our concern has to be with the process of taking a limit as one endpoint moves to infinity.

5 Spectral Density

Supposing that a and b are both finite, defining an interval in which p is not zero and q is not singular, we can suppose that the Sturm-Liouville system exists for that interval. Thus there is a sequence of eigenfunctions ψ_i, with eigenvalues λ_i, which allows the expansion of an arbitrary function f:

$$f(x) \quad = \quad \sum_{i=0}^{\infty} c_i \psi_i,$$

The completeness of such a basis $\{\psi_i\}$ can be exhibited through the general validity of Parseval's equality

$$\int_a^b |f(x)|^2 dx \quad = \quad \sum_{i=0}^{\infty} |c_i|^2,$$

which we can write in the more symbolic form

$$(f, f) \quad = \quad \sum_{i=0}^{\infty} |(\psi_i, f)|^2,$$

Now, use the bracket to evaluate these inner products:

$$\frac{1}{\lambda - \lambda^*}\{[f,f](b) - [f,f](a)\} \quad = \quad \sum_{i=0}^{\infty} \frac{|[f,\psi_i(b) - [f,\psi_i](a)|^2}{|\lambda - \lambda_i|^2},$$

The point is that all expansion formulas use parentheses, which we can turn into brackets at will by using Green's formula.

To simplify this expression we should like to nullify its dependence on the point b, and to standardize its dependence on the point a. Independence from b will be particularly important in taking the limit as the right endpoint recedes to infinity. Although the elimination of b cannot be achieved for all functions f, we can commence by selectively applying the formula to functions lying in the null space of the bracket at the right endpoint. We have already seen that this leads to the Titchmarsh-Weyl m function, and will moreover leave the left-hand side of the equation free of an explicit dependence on b.

Removal of b from the right-hand side of the equation can be accomplished by the selection of the boundary conditions which the Sturm-Liouville eigenfunctions are to satisfy, which could include the requirement that their brackets with f (or its real and imaginary parts) vanish. While it is necessary to verify that we are at liberty to make such a requirement, we nevertheless have the means of removing the explicit dependence on b from the right-hand side of the equation.

Standardization of the form of the right-hand side at the left-hand boundary point a can be accomplished by employing the remaining Sturm-Liouville boundary conditions together with the arbitrariness still resident in the definition of the m function, that it is the coefficient of only one of the initial-value basis functions.

Weyl's line of reasoning was to insist that the function f meet a real boundary condition at b, which of course ensures that $[f,f](b) = 0$. Then he required that the Sturm-Liouville system meet the same boundary condition as f, which is tantamount to requiring that

$$[f,\psi_i](b) \quad = \quad 0,$$

To meet the corresponding requirement at a, we require that ψ satisfy a real initial value, and that

$$[\psi,\psi_i](a) \quad = \quad 0,$$

so that

$$[f,\psi_i](a) = [\varphi,\psi_i](a) = r_i.$$

This proportionality constant r_i, has the significance that the initial-value basis function ψ starts out from a unitary initial value in the boundary value space, so that $[\varphi,\psi] = 1$, while the basis functions ψ, are normalized to unity in the Hermitian metric in the solution space $(\psi_i,\psi_i) = 1$ *Then r_i has the significance that it is the initial amplitude of a real normalized solution of the differential equation over the interval a, b.* When we are dealing with a continuum wave function which has an

asymptotically constant amplitude, a quick way to obtain this proportionality is to solve the initial-value problem with unit initial amplitude, then take the reciprocal of the asymptotic amplitude. The actual value will be this amplitude multiplied by the length of the interval, if the length is long enough, any contributions due to the part of the solution near the origin will be washed out.

We are now ready to write the Parseval equation in the form

$$\frac{m - m^*}{\lambda - \lambda *} = \sum_{i=0}^{\infty} \frac{r_i^2}{|\lambda - \lambda_i|^2}$$

which is valid for those values of $m(b)$ which comply with all the requirements which we have set down, and the coefficients r_i, and the eigenvalues λ_i, are calculated with respect to a suitable Sturm-Liouville problem for each value of b.

The most effective technique which seems to have been found for passing to an infinite interval with the Parseval equality is to take it as an approximation to a Stieltjes integral

$$\frac{m - m^*}{\lambda - \lambda *} = \int_{-\infty}^{\infty} \frac{d\rho(\mu)}{|\lambda - \mu|^2}$$

wherein the spectral distribution function $\rho(\mu)$ is approximated by a step function whose increment at the eigenvalue λ_i is r_i^2. There are three logical possibilities at a point μ_0 as the interval becomes infinite

1. $\rho(\mu)$ has a discontinuity at μ_0,
2. $\rho(\mu)$ is continuous but not constant at μ_0,
3. $\rho(\mu)$ is continuous and constant at μ_0

In the first case we say that μ_0 is a point in the discrete spectrum of $\mathcal{L}$, in the second case we say that it is a point in the continuous spectrum of $\mathcal{L}$. μ_0's belonging to the third category are not spectral points. The classification agrees with the classification obtained from the resolvent in operator theory.

It cannot be emphasized too strongly that there are *two* aspects of the spectrum of the finite Sturm-Liouville problem which enter into the determination of ρ: one is the number of eigenvalues in any unit of interval, but the second is the *value over the origin* of the normalized eigenfunctions.

There is absolutely nothing in the theory which requires the spectral distribution function to be differentiable, yet it possesses this remarkable property in a majority of the examples of practical interest We could write, in such an event,

$$\frac{m - m^*}{\lambda - \lambda *} = \int_{-\infty}^{\infty} \frac{\rho' d\mu}{|\lambda - \mu|^2}$$

and even

$$\text{Im } (m) = \text{Im} \left\{ \int_{-\infty}^{\infty} \frac{\rho' d\mu}{\lambda' - \mu} \right\}.$$

The derivative ρ', when it exists, is called the *spectral density function*. A point to be borne in mind is that the m function is analytic in its domain of definition, and therefore might be expected to be differentiable. But remember that we are now talking about the boundary value, on the real axis, of a function which is not immediately defined there. It is therefore a matter of individual cases as to whether the real axis is a natural boundary, or whether the m function can be continued up to, and across, the real axis. We recall that this deficiency, of not being defined for real eigenvalues, which is shared by functions obtained from the bracket, was the motivation for working with a complex eigenvalue parameter at the outset.

If we have an analytic spectral distribution function, we are extremely fortunate, because it is possible to incorporate a great deal of complex analysis in the study of our differential operators. In particular, an analytic continuation of the spectral density may often be made across the real axis, into a region which is not accessible by the mere solution of a differential equation. In addition there are dispersion relations which can sometimes be written, which are very much related to questions of causality in some of the physical applications.

Since the spectral density is so closely related to the Weyl-Titchmarsh m function, the calculation of the latter can be used as a numerical technique for the location of the eigenvalues of a differential equation. Poles correspond to points in the discrete spectrum, whereas branch points delimit the intervals occupied by the continuous spectrum.

Traditional studies of the continuum have been noteworthy for their lack of imagination, taking it for granted that a continuum must be highly amorphous. For some potentials, notably the constant potential of a plane wave or even the Coulomb potential of the hydrogen atom, there is little which is remarkable about the spectral distribution function. Once the potential shows a little variability, however, it is found that the spectral density oscillates sedately, passing through a sequence of maxima and minima, whose sharpness and amplitude vary with the potential. Such oscillations imply possible poles in the m function the moment an analytic continuation is made across the real axis onto the unphysical sheet. In turn the poles encountered during the analytic continuation together with their residues may provide a very concise summary of the properties of the differential equation and its solutions, mathematically accessible through a Mittag-Leffler expansion of the m function.

It is not clear whether such a summary should be carried to the extent of attempting to construct an eigenfunction expansion based on the complex poles of the Titchmarsh-Weyl function. Most of the difficulty to be encountered in such an enterprise stems from the fact that an analytic continuation of the wave function is not necessarily a solution of the analytic continuation of its differential equation, or that it would be the same solution even if it satisfied the differential equation This discrepancy produces Stokes's phenomenon in the analytic continuation of a solution around a singular point of the coefficients of a differential equation. Indeed, the term "unphysical sheet" recognizes the fact that it contains functions which are not directly accessible as the solutions of Schrödinger's equation, but rather indirectly deduced through the process of continuation.

Sometimes it is possible to construct a biorthogonal set of functions employing the complex poles on the unphysical sheet, and sometimes it is possible to give a physical interpretation to the wave function on the physical sheet which is associated with one of the complex poles by ignoring the distinction between sheets. These associated wave functions tend to grow in the worst possible fashion, and so are possessed with an exponential growth which is too drastic to be accounted for by delta-function normalization. However, they do play a role in time-dependent problems, which gives an interpretation through the formation of wave packets, in which the real part of the pole signifies a resonance peak while the imaginary part is the reciprocal half-life for the decay of a transient state.

It is a mistake to treat the complex poles as energy levels, supposing that they are on the same footing as the poles on the real axis, which determine the bound states. Especially, they should be associated with wave functions with extreme caution. Still, when they are employed in a correct way the complex poles, together with branch points and other singularities, summarize the differential equation from which they arise, in the way that an analytic function is always determined by its singularities.

6 Continuation in the Complex Eigenvalue Plane

The exact nature of the spectral density depends to a considerable extent on the potential employed. It would seem that some hesitation has arisen in the application of S-matrix techniques on account of a lack of familiarity with the characteristics to be expected of differing potentials. For example, square well potentials, and in general those potentials which are cut off, oscillate, or have abrupt changes, tend to have a rich assortment of complex poles near the real axis in the complex energy plane. Potentials which vary smoothly, for example those which behave as a power of the distance, may have only an essential singularity at infinity, as happens for the pure Coulomb potential. Exponentially decreasing potentials show an assortment of real poles on the second sheet, without having any strictly complex poles. It would appear that this is a phenomenon relatively familiar to acoustical or electrical engineers, for whom exponential horns have a special significance. Yet considerable consternation occurred among physicists when this potential was first encountered in S-matrix theory.

Potentials which offer definite but not insurmountable barriers to particle motion have a much better developed pole structure in the spectral density function than those which are monotonic and never rise above their asymptotic value. Potentials created by a configuration of a few fixed atomic nuclei with their Coulomb potentials do not show such behavior, but the Stark effect in atomic spectroscopy is an excellent example of a system in which, in the idealized case, the potential even drops to negative infinity at large distances. When the electric field strength is reasonably large the barrier to ionization of the system is not particularly great, giving continuum states concentrated around the perturbed energy levels, but with an appreciable level width.

Another more esoteric example is to be found in the Dirac equation, in the physically not very realistic case in which the rest mass and the binding energy of the

particle are comparable. Here the Klein paradox enters into play, wherein it is found that an appreciable tunneling is possible between positive and negative energy states. The result is that increasing potentials, such as the harmonic oscillator potential, have a continuum of eigenvalues rather than the well-defined discrete spectrum which we find in the non-relativistic oscillator described by the Schrödinger equation. However, as the rest mass increases in relation to the strength of the quadratic potential well, it is found that the continuous spectrum becomes more and more concentrated, approaching more and more to a discrete spectrum in appearance.

Square well potentials, singly or in combination, afford some of the simplest examples because of the ease with which explicit solutions for either the Schrödinger equation or the Dirac equation may he formed and applied to the determination of the spectral distribution function. Moreover it is possible to arrange some very illuminating combinations such as an exponential well or a Yukawa well. A notch a finite distance from the origin was Gamow's original model for the radioactive decay of a nucleus by the emission of an alpha particle.

A clarification of the exponential well would be especially pertinent because it was the model in which the false poles of the S-matrix made their debut. With such a potential we are not too far from the result known to electrical engineers that the best impedance match between two dissimilar lines is to be had by giving the joining section the geometric mean of the two impedances which have to be matched.

One slight caution which must be observed in building up limiting approximations to potentials is that a limiting sequence of poles is likely to turn into a branch cut in the complex plane of the spectral density, giving the limiting potential ralher different properties than those of its approximations For example, cutoff potentials seem to have a different singularity structure from those which are strictly analytic Analytic continuation is a highly sensitive and unstable numerical procedure, for which relativly insignificant alterations of the continued function in one region can produce exaggerated effects in another As a result, poles near the cut line and reasonably close to the origin have a better chance of being detected, while the behavior in remoter areas is much more uncertain.

It would seem that numerical problems of this nature have held back the large-scale description of scattering processes through a Mittag-Leffler expansion of the spectral density, even when the analyticity of the m function is already conceded and the possibility of its continuation is not in doubt. Nevertheless, both the Schrödinger and the Dirac equations can be analyzed, and many general conclusions obtained, by working with carefully chosen piecewise constant potentials.

A 2×2 matrix notation is admirably suited for discussing one-dimensional problems. For the Schrödinger equation, we would write

$$\frac{d}{dx}\mathbf{Z} = \begin{pmatrix} 0 & 1 \\ V-E & 0 \end{pmatrix}\mathbf{Z}$$

taking $\mathbf{Z}$ as a matrix containing two linearly independent solutions. By introducing the variables

$$\varphi = w(V-E)^{1/2}, \quad \sigma = (V-E)^{-1/2}$$

the solution matrix of the equation assumes the form

$$\mathbf{Z}(w) \quad = \quad \begin{pmatrix} \cosh\varphi & \sigma \sinh\varphi \\ (1/\sigma)\sinh\varphi & \cosh\varphi \end{pmatrix}$$

In a similar manner, if we take the Dirac equation to have the form

$$\frac{d}{dx}\mathbf{Z} \quad = \quad \begin{pmatrix} 0 & m_0 - (V-E) \\ m_0 + (V-E) & 0 \end{pmatrix} \mathbf{Z}$$

the substitutions

$$\varphi = w[m_0^2 - (V-E)^2]^{1/2}, \quad \sigma = \left(\frac{m_0 - (V-E)}{m_0 + (V-E)}\right)^{1/2}$$

lead to a solution matrix of just exactly the same form.

Multiplying together the solution matrices belonging to the constant segments is the way to resolve a piecewise constant potential, and even a good way to approximate a more arbitrary potential. Although the result can be quite explicit, increasingly cumbersome algebraic expressions arise when there are more than a very few segments. Their complexity is even more severely compounded by calculating the bracket of two solutions. Especially because the numerical behavior is easily hidden in a complicated formula, it is helpful to have some simpler estimates available.

When f represents the bounded solution, while ψ and φ are the unbounded basis solutions, an approximation may be obtained by dividing the defining equation

$$f \quad = \quad \varphi + m\psi$$

by ψ. Because the left-hand side would become negligible in the limit, there remains the estimate

$$m \quad = \quad -\lim_{x\to\infty} \frac{\varphi(x)}{\psi(x)}.$$

As no bracket is involved, it is a formula which is algebraically much simpler than the complete expression would be. However, it is only valid for limit point potentials, and not where the limit circle arises.

The asymptotic form for the solutions may already be deduced once the coefficients of the differential equation are nearing their limiting values. Regarding the coefficient matrix as constant from that point onward, the solution matrix can be factored in the form

$$\begin{aligned} \mathbf{Z}(w) \quad &= \quad \begin{pmatrix} \cosh\varphi & \sigma\sinh\varphi \\ (1/\sigma)\sinh\varphi & \cosh\varphi \end{pmatrix} \begin{pmatrix} A & C \\ B & D \end{pmatrix} \\ &= \quad \begin{pmatrix} A\cosh\varphi + B\sigma\sinh\varphi & C\cosh\varphi + D\sigma\sinh\varphi \\ (A/\sigma)\sinh\varphi + B\cosh\varphi & (CA/\sigma)\sinh\varphi + D\cosh\varphi \end{pmatrix} \end{aligned}$$

where φ corresponds to the width of the asymptotic segment.

This matrix can be given a more precise appearance by defining

$$\begin{aligned} r &= (A^2 - B^2\sigma^2)^{1/2}\,, \quad & \delta_1 &= \operatorname{arctanh}\,(-B\sigma/A) \\ s &= (C^2 - D^2\sigma^2)^{1/2}\,, \quad & \delta_2 &= \operatorname{arctanh}\,(-D\sigma/C) \end{aligned}$$

and eventually,

$$\mathbf{Z}(w) \quad = \quad \begin{pmatrix} r\,\cosh\,(\varphi+\delta_1) & s\,\cosh\,(\varphi+\delta_2) \\ (r/\sigma)\,\sinh\,(\varphi+\delta_1) & (s/\sigma)\,\sinh\,(\varphi+\delta_2) \end{pmatrix}.$$

Combining this form of the solutions with the estimate for the m function, we obtain

$$m \quad = \quad -(s/r)\exp(\delta_1 - \delta_1).$$

This is the formula which establishes the closest connection between the theory of differential equations and the S-matrix theory of quantum mechanics, by exhibiting the identity of the S-matrix and the spectral density in a way which clearly shows the assumptions involved. In one dimension, the S-matrix is a single number, whereas in general it is a matrix. However, the spectral density also generalizes to a spectral matrix when there is a system of coupled differential equations, so that the connection can be maintained quite generally.

The assumptions at stake consist in having a limit point differential equation, and having m defined for real eigenvalues Then the formula can even be used to estimate m from a purely real wave function because r and s each have simple interpretations – the asymptotic amplitudes of their wave functions Thus may be obtained the factor r_i^2 which is needed in the Stieltjes integral which defines the spectral distribution function.

It is interesting that m is approximated by a quotient of amplitudes rather than by the square of a single asymptotic amplitude. The implication is that the two amplitudes are reciprocals, which is the relationship by which the poles of the S-matrix on the unphysical sheet are interpreted in terms of the zeros of the complementary wave function on the physical sheet. This in turn has promoted the interpretation of real poles on the unphysical sheet as "antibound" states, whose "wave functions" grow in the worst possible way.

All these concepts need to be employed with considerable caution, because several things are being taken as equivalent which in reality only coincide under explicit but hardly all-inclusive circumstances. For example, the square of the amplitude of the finite Sturm-Liouville solutions only enters in the approximation of the spectral *distribution*. Additional requirements are the assumption of differentiability and a dispersion relation to arrive at the special spectral *density*. Finally an amplitude and the reciprocal of the complementary amplitude enter through an approximation to the m function, and define the Jost function, which is the S-matrix for one dimension.

7 One-Dimensional Relativistic Harmonic Oscillator

The most dramatic visualization of the spectral density arising from a continuum is to graph the wave functions side by side according to their energy dependence, normalized with their asymptotic amplitude unity. The resulting amplitude at the origin portrays the spectral density. Supposing that the amplitude at infinity signifies the strength of a current, the idea of a resonance or antiresonance surely depends on the observation that at some energies a unit current produces a maximum amplitude over the origin, while at other energies this amplitude will be at a minimum. What remains is to associate the maxima and their intervening minima with poles and zeros in the complex plane, complying with the idea that an analytic function is defined by its poles and their residues.

The process is illustrated in the accompanying figures by a series of computer-generated graphs The differential equation selected is the Dirac equation for a one-dimensional harmonic oscillator extending over the doubly infinite interval. Because the solutions are either even or odd the corresponding initial conditions can be chosen and the display of the solutions restricted to a single half interval.

Nikolsky [17] made the original investigation of the Dirac harmonic oscillator in 1930, finding its spectrum to be a continuum extending over the whole infinite interval He observed that although the spectrum was infinite in extent, it was not uniform, some wave functions having smaller asymptotic amplitudes than others. In 1935, Postepska [18] used the WKB method for a more detailed study of the solutions, examining the sharpening of the spectrum in the nonrelativistic limit. Motivated by a perturbation calculation of Sewell [19] which purported to exhibit the relativistic shift of the harmonic oscillator energy levels, Titchmarsh [20] analyzed the migration of the poles of a Green's function into the complex plane as a consequence of varying the velocity of light, finding an exponential variation in their distance from the real axis.

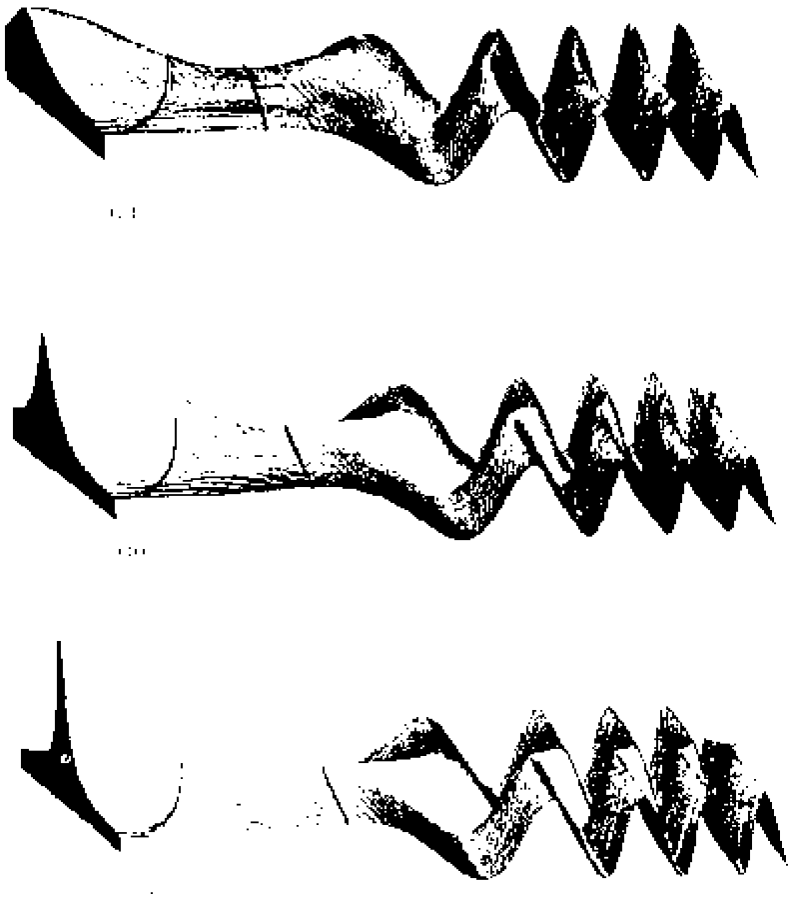

Figure 1: Solutions to the Dirac equation for a one-dimensional harmonic oscillator. A single curve shows the even, positive energy solution, with markers indicating the classical turning points. The energy eigenvalue varies from m_0 in the foreground to $m_0 + 1$ in the background, an interval containing a single resonance. (a) Small rest mass, (b) intermediate rest mass, (c) large rest mass. Note the increasing sharpness of the resonance with mass, likewise the increasing abruptness of the 180^o phase shift over the interval. The wave functions are normalized to unit asymptotic amplitude.

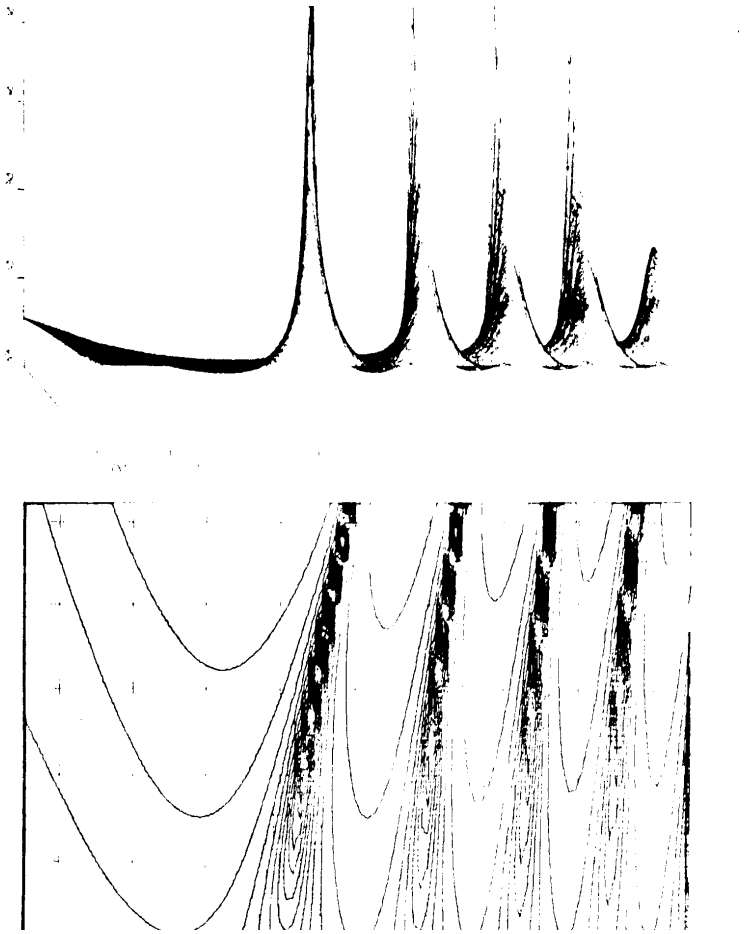

Figure 2: Amplitude at the origin for wave functions having unit asymptotic. amplitude. The horizontal axis represents energy, the depth coordinate rest mass which is zero in the foreground. (a) Perspective view, (b) contour map. In the shaded region, the amplitude is greater than unity. The inclination of the contours results from measuring the energy from zero rather than m_0, while their curvature is a relativistic effect. The "islands" at high mass are spurious, arising from a finite contour grid.

In the course of the three diagrams which constitute fig 1, we pass from a very light rest mass, which provides a very broad resonance, through a moderate resonance, and finally to a somewhat larger rest mass which produces a rather sharp resonance. In all cases the wave function has been normalized to unit amplitude at infinity, so that its amplitude over the origin will allow the poles of the spectral density to be located.

The classical turning points, both for positive and for negative energy states, have been indicated. As with the Schrödinger equation, these are points of inflection for the wave function, and mark the transition between a region of oscillatory behavior for the wave function and a region of exponential behavior. As the rest mass increases, the exponential region is enlarged, which makes the obtaining of a wave function with a large amplitude within the potential well increasingly difficult. In the limit, the nonrelativistic harmonic oscillator is seen to be an extraordinarily sharp resonance state, with essentially only one energy at which an interior amplitude is possible.

It is possible to observe quite clearly some other phenomena associated with resonance, for example, the fact that the asymptotic wave function undergoes a 180^o phase shift on passing the resonance while gradually increasing the energy As the resonance narrows, the transition is increasingly abrupt.

In the two diagrams comprising Fig 2 we summarize the spectral density with variation of energy and rest mass of the particle. Figure 2a is a perspective view of the function; Fig. 2b is a contour plot. The convergence of the spectral density to delta functions is quite evident.

Once a series of examples has been examined, the convenience of the m function in the solution of differential equations and in the presentation of the properties of those solutions can be appreciated. The origin of this function is mostly mathematical, arising in a natural way from Green's formula and the relationships between inner products in a general function space and in the space of boundary values for a differential operator. It is reassuring to see that it is so closely related to the S-matrix, which arose from highly physical considerations. Nevertheless the motivation was quite similar, to express the results of experiment directly in terms of initial conditions and physically observable quantities, without encountering too much detail about the actual dynamical processes.

8 Survey

A number of perplexing situations which have arisen during the course of development of quantum mechanics have a very nice interpretation in terms of the complex poles and other singularities of the spectral density. Foremost among these is the question of the convergence of perturbation theory, let alone its very meaning in the context of a continuous spectrum.

Perturbation theory, even in the variant forms in which it is sometimes presented, inevitably consists of formulas which describe a purely real process carried out on purely real data. Naturally the procedure involved cannot account for the migration of a pole away from the real axis out into the complex plane. Moreover, it seems

to be the general rule that the movement of the poles out to infinity from their real unperturbed values depends exponentially on the perturbation parameter, in a way which introduces an essential singularity at zero strength. Power series expressions for the perturbed eigenvalues cannot work, leaving asymptotic formulas as the best for which we can hope.

Symmetry and degeneracy do not play any important role in one-dimensional problems, but the spacing of the eigenvalues and relative location of the complex poles constitute an important consideration in assessing these characteristics of separable higher dimensional problems. It is therefore interesting to consider the implications of the Weyl-Titchmarsh theory for symmetry and degeneracy for those potentials amenable to analysis through separation of variables. The theory of the universal symmetry group, for example, was based on the construction of ladder operators for each of the separation coordinates.

Certainly any separation equations which lead to purely bound states will be amenable to a Sturm-Liouville treatment which can be extended in the limit to a complete orthonormal family of eigenfunctions. As this family is naturally ordered by the size of the eigenvalues and the number of nodes of the eigenfunctions, there is not much difficulty to imagine ladder operators for the assemblage, both raising and lowering the eigenvalue. Continuum states will create complications, particularly if the m function has singularities other than poles near the real axis, but in general terms can be fitted into the same scheme.

However, it will hardly be expected that there will be any regular relationship among the eigenvalues. Whenever such a relationship might be discovered, it would certainly be possible to modify it slightly by a small modification in the potential. Thus, the orderly spectra should constitute at the most a very small sample among the possible spectra.

Dealing with continuous spectra, which realism insists must occur in the preponderant majority of cases, we would expect the eigenvalues to be replaced by the complex poles in the spectral density function, which are likely to be countable in number, although not directly associated with a complete orthonormal set of eigenfunctions. Especially when the poles lie very close to the real axis, they will constitute the closest approach to an assortment of eigenvalues which we are likely to obtain. By a more careful analysis it can be made plausible that here, too, the actual procession of poles can just about be made to order, making it a vain hope that there would be some general principle of nature which would regulate the location or spacing of the poles.

It is not excluded that such regularity might dominate the equations describing fundamental processes, such as the direct interactions of elementary particles, but it seems hopeless to expect it to persist in the equations summarizing more complicated configurations.

In a realistic multidimensional problem, the way it which these poles, be they real or complex, are to be combined once they arise from the separated constituents of Schrödinger's equation will depend on the individual cases. That is, the expression for the complete eigenvalue will depend rather much on the separation constants which arise, how they enter into the separated equations, and how the total energy

is functionally dependent on them. Nevertheless it would seem that any degeneracies or approximate degeneracies which might exist would have an overwhelming tendency to be statistical accidents. Supporting this view is the observation already made that slightly different separation potentials would have slightly different spectra, and moreover these spectra could be slightly different in any way which we might choose. It is not even necessary to speculate on the modifications which might lead to the same result of slightly deviating spectra, but through a nonseparable modification to the potential. Therefore the distribution of energies, and hence apparent degeneracies or near degeneracies, would seem to be alterable in a completely arbitrary manner.

It is therefore clear that it is not the mere existence of ladder operators, capable of mapping one eigenvalue into another, which is the determining factor in establishing accidental degeneracy. It is necessary that each of the individual separation spectra has a strict regularity, and that the raising of eigenvalues in one separation coordinate can be exactly balanced by a lowering in another.

Such reasoning, it would seem, completely dissipates any further hope for a universal symmetry group. At the same time it points a direct finger at the relationship between unitary and canonical transformations as seen from the theory of operators on Hilbert space.

If we have lost a possible application of group theory in quantum mechanics through the loss of the universal group, we have at least gained a new source of interest through the intervention of the symplectic group in such an interesting way in the space of boundary conditions, much as the unitary group enters into the space of wave functions.

Some new perspectives in the relationship of symmetry groups and dynamical groups to the spectrum of the Hamiltonian emerge from the complex approach to eigenvalue theory One of these arises in Regge pole theory, because the angular momentum is treated as a complex variable, rather than being restricted to the eigenvalues of the total angular momentum. Presumably there exists a complex eigenvalue theory for the angular momentum operators as well as for the Hamiltonian, with a corresponding representation theory. Some studies have been made of this phenomenon, which requires the infinite-dimensional nonunitary representations of the three-dimensional rotation group. It is a speculative area, just as the attempts to fit the nonphysical eigenfunclions of the Hamiltonian into a Hilbert space theory are somewhat peripheral to the main lines of quantum theory. Nevertheless some interesting relationships may repay still further study.

Finally, and most important, the concept of square integrability should lose some of its mysterious aloofness. If it is seen to be an auxiliary concept rather than a first principle, the process of integrating the Schrödinger equation or the Dirac equation becomes an ordinary exercise in differential equation theory. Thus the use of differential equations in physics should be no different than in any other branch of engineering.

One point which perhaps is not as much appreciated as it should be, and which emerges from a careful theory of differential equations, is *the way in which the eigenfunctions of the differential equation operator may be used to form an eigenfunction expansion of Hilbert space without ever being required to belong to Hilbert space them-*

selves. Only in this way can we have continuum wave functions, and at the same time a probabilistic interpretation with normalizable functions, which evidently have to be wave packets, and not individual eigenfunctions. Such is the compromise between probability theory and differential equation theory which seems to be required.

Much remains incomplete in this survey of quantization as an eigenvalue problem, particularly since we have fostered the idea that an "eigenvalue problem" consists in selecting those solutions of a differential equation which look "interesting." At least in one dimension it is not too difficult to produce an assortment of interesting possibilities from which to make a selection. It is also possible to make some well-founded evaluations of the situation prevailing for partial differential equations, when more than one dimension has to be considered.

Square integrability is a valid quantizing principle, but must be applied to the total wave function. Ordinary continuum wave functions are not expected to be square integrabte, and the probability interpretation must be abandoned in favor of probability currents or of relative probability. Only if the growth of the wave function is still too strong for these localized requirements must it be rejected.

Finiteness as a quantizing principle seems to make its appearance in separated equations, and is related to the requirement that the total wave function have some acceptable probabilistic interpretation.

The total wave function for a separable equation is a product of individual wave functions, which leads to a specialized form of Green's formula. The one-dimensional formula can produce a finite bracket from very large arguments because it involves a difference of a product, whereas the bracket for separated equations involves the arguments directly as factors. Hence, there is an additional requirement for their finiteness which is not relevant to an isolated one-dimensional wave equation. The difficulty lies in the more complicated structure of the multidimensional bracket, which violates our naive assumptions. It is not unlike the way in which an element of area transforms as a vector product of the edge elements, rather than the simple product which we tend to assume carelessly.

The one instance where square integrability rather than finiteness is decisive occurs in the radial equation of the Dirac hydrogen atom. To fit this into the explanation just given would require us to investigate Green's formula for the separable Dirac equation, which is surely somewhat different from the Schrödinger Green's formula.

Directly or indirectly, the insights which produced quantum mechanics have already sustained the. mathematical sciences for 50 years, with every indication of continuing to exert their influence. What began as a mixture between a calculus for combining tables of spectral lines and a differential equation generalizing classical mechanics in the direction of wave optics has dominated our entire thinking about physical reality, and has still not ceased shaping and guiding much of the world's intellectual effort. The theory of operators on Hilbert space, not to mention the theory of rings of operators, was rudely forced beyond the mathematicians' convenient restrictions to bounded operators and continuous mappings by the necessity of solving the Schrödinger equation for realistic systems. The foundations of probability theory had to be given a sharper form before accurate statements could be made about the

probabilistic interpretation of the wave function and about the theory of measurement. In recent years numerical methods have been refined and computer technology stimulated, in part to integrate the Schrödinger equation. Even the arcane lore of group representation theory, which flourished at the beginning of the century, was resurrected and adapted for continuous groups to allow progress in the quantum mechanics of many-particle systems. Yet even after all this activity, our understanding of quantization as an eigenvalue problem has barely begun.

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