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The Factorization Method

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The factorization method is an operational procedure which enables us to answer, in a direct manner, questions about eigenvalue problems which are of importance to physicists. The underlying idea is to consider a *pair* of first-order differential-difference equations which are equivalent to a given second-order differential equation with boundary conditions. For a large class of such differential equations the method enables us to find immediately the eigenvalues and a manufacturing process for the normalized eigenfunctions. These results are obtained merely by consulting a table of the six possible factorization types.

The manufacturing process is also used for the calculation of transition probabilities.

The method is generalized so that it will handle perturbation problems.

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1. Introduction

THIS report deals with a new technique for solving eigenvalue problems as they most frequently appear in wave mechanics and in Maxwell's theory with imposed boundary conditions. Special attention is given to quantum theory where the field of applications is very wide.

To introduce the idea behind the method let us briefly mention a subject which is often discussed: the analogy between Maxwell's and Dirac's equations. Both are linear systems of equations and each of them contains partial derivatives of the first order. Both Maxwell's and Dirac's equations are Lorentz invariant. We may remark, in passing, that in the case of Maxwell's equations the linearity may be an over-simplification which leads to the difficulties with infinite self-energies. But, if we consider only regular solutions, as we shall, we may ignore this difficulty.

Historically, the Maxwell and Dirac equations were each preceded by a scalar theory. In the case of Dirac's theory the preceding one was the Schrödinger theory, which is still applied to a wide range of quantum-mechanical problems. The scalar theories lead to one partial differential equation of the second-order containing the Laplacian or d'Alembertian. As these names indicate the study of such scalar equations is an important chapter in the mathematics of the nineteenth century. It led to potential theory, to Legendre, Laguerre, Jacobi, Tchebycheff, and Hermite polynomials and to Bessel functions, all of which form a part of mathematical physics which was completed by the time scalar field theories were being replaced by vector, tensor, and spinor theories.

Thus the technique of solving Maxwell's and Dirac's systems of equations became modeled upon the scalar theories. This is especially evident in the case of Maxwell's equations. There the usual procedure is to introduce a vector and a scalar potential and then obtain four equations of the type studied in a scalar theory. If you think about an application of Maxwell's theory to a wave guide with rectangular or circular cross section, or to an antenna, you see how the boundary conditions finally lead us to a set of ordinary differential equations of the second order.

In many respects the situation is even simpler in wave mechanics. There the boundary conditions are more intimately connected with the differential equation itself and they usually mean single-valuedness and quadratic integrability.

Thus, both in electromagnetic theory and in quantum theory, we are lead to equations of the type

$$(d^2y/dx^2)+r(x, m)y+\lambda y=0.$$

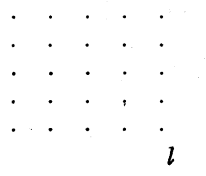
Here $r(x, m)$ is a function which characterizes the particular problem. We shall assume m to be a non-negative integer

$$m=0, 1, 2, \cdots$$

which is gained through the process of separating variables; its value is restricted by the boundary conditions. In most cases the boundary conditions require further that λ have discrete eigenvalues

$$\lambda_0, \lambda_1, \lambda_2, \cdots \lambda_l \cdots.$$

Thus the typical eigenvalue problem can be represented by a lattice of points in the (l, m) plane



For every line connecting the lattice points and parallel to the m-axis there exists a λ_l. For every point on the lattice there exists a function $y_l{}^m(x)$ satisfying some boundary conditions.

All we have done so far is to recapitulate an idea familiar to every theoretical physicist; it is a cornerstone of mathematical investigations of physical problems.

1.1 Characterization of the factorization method

The classical method consists in first finding general solutions of the differential equation and then determining the special values of λ which allow these solutions to satisfy the boundary conditions; thus the function $y_l{}^m(x)$ belonging to each point on the lattice is obtained. This function can then be normalized and finally used, for example, to calculate transition probabilities.

The factorization method outflanks and unifies the historical approach. This new method leads directly to the eigenvalues and to a manufacturing process for the normalized eigenfunctions. The manufacturing process itself can then be used to calculate the transition probabilities.

The factorization method either treats the original first-order differential equations directly or replaces the second-order differential equation by an equivalent pair of first-order equations of the form

$$\left\{k(x, m+1)-\frac{d}{dx}\right\}Y_l{}^m=[\lambda-L(m+1)]^{\frac{1}{2}}Y_l{}^{m+1}$$

$$\left\{k(x, m)+\frac{d}{dx}\right\}Y_l{}^m=[\lambda-L(m)]^{\frac{1}{2}}Y_l{}^{m-1}.$$

These equations can be obtained from a table of all possible factorizations. There are only six possibilities, and even these six are not independent. Once the proper factorization is found from the table, the eigenvalues and the manufacturing process for the eigenfunctions can be written down immediately.

The table can be used in other ways. For example, if the eigenvalues are already known, corresponding possible potential functions can be found from the table.

What is the range of validity of this new method? Let us concentrate our attention on wave mechanics. There we find some "pure" problems, by which we mean those which can be solved rigorously without the use of any perturbation or numerical procedure. All these pure problems can be solved quickly and in a unified way by the factorization method. Moreover, each of the six possible factorization types has a physical image in Maxwell's theory, or in quantum theory, or both.

Yet "purity," though a desirable phenomenon, is a rare one and as science and its techniques develop, the number of non-pure cases built around each pure case constantly increases. It is therefore gratifying to know that the factorization method can be generalized to handle perturbation problems. In some cases, as in the Stark effect, the method leads us more quickly than any other to the solution.

The factorization method owes its existence primarily to a paper by Schrödinger (41).[1] His ideas have since been considerably generalized (21, 22, 24, 25, 27, 28, 32, 42, 43, 46). There were, however, earlier indications of the idea in Weyl's (51, p. 231) treatment of spherical harmonics with spin and Dirac's (9) treatment of angular momenta and the harmonic oscillator problem. More recently an alternative to the factorization method has been given by Inui (29).

Almost any section of this report can be read once the basic ideas in Chapter 2 have been understood.

2. Theory of the Factorization Method

In this capter we begin by assuming that an equation has been factorized and then proceed to demonstrate, by developing five theorems, the consequences of this fact. We shall see that the factorizing of an equation enables us to write down immediately the desired eigenvalues and the normalized eigenfunctions.

In the next chapter we shall show how to find the factorization of a given equation. In fact, the problem of factorizing will be reduced to one of consulting a table of only six general types. This table, with many important special cases, is given at the end of the paper.

Thus this chapter and the next contain only the *idea* and *technique* of the factorization method on which the examples in the remainder of the paper are based. Almost any subsequent section can be read, without loss of continuity, immediately after reading Chapter 2.

2.1 Standard form

To systematize our procedure we shall always transform the considered differential equation into the standard form

$$(d^2y/dx^2)+r(x, m)y+\lambda y=0 \qquad (2.1.1)$$

where the parameter $m=m_0, m_0+1, m_0+2\cdots$; here we will take $m_0=0$ but, as we will see, this assumption does not affect our final conclusions.

Such a transformation is possible if, in the original form

$$\frac{d}{d\theta}\left(p\frac{dP}{d\theta}\right)+qP+\lambda\rho P=0,$$

the functions p, ρ are never negative and ρ/p exists everywhere. The transformation connecting these equations is (6, p. 250):

$$y=(p\rho)^{\frac{1}{2}}P, \quad dx=(\rho/p)^{\frac{1}{2}}d\theta. \qquad (2.1.2)$$

[1] References given in parentheses are placed at the end of this article.

2.2 Definition and fundamental idea; Theorem I

We say that Eq. (2.1.1) can be factorized if it can be replaced by *each* of the following two equations:

$$ {}^{+}H^{m+1}\,{}^{-}H^{m+1}y(\lambda, m)=[\lambda-L(m+1)]y(\lambda, m) \quad (2.2.1a) $$

$$ {}^{-}H^{m}\;\;{}^{+}H^{m}\;\;y(\lambda, m)=[\lambda-L(m)]y(\lambda, m) \quad (2.2.1b) $$

where

$$ {}^{\pm}H^{m}=k(x, m)\pm(d/dx). \quad (2.2.1c) $$

The dependence of y on x has been suppressed. Just how the ${}^{\pm}H^{m}$ and $L(m)$ are found in a given problem will be considered later (Sec. 3.1).

We should note that (2.2.1a) can be obtained from (2.2.1b) by interchanging the H operators, and changing m to $m+1$ except in the function $y(\lambda, m)$.

The fundamental idea of the factorization method can now be established:

Theorem I. If $y(\lambda, m)$ is a solution of our differential equation then

$$ y(\lambda, m+1)={}^{-}H^{m+1}y(\lambda, m) \quad (2.2.2a) $$

$$ y(\lambda, m-1)={}^{+}H^{m}y(\lambda, m) \quad (2.2.2b) $$

are also solutions corresponding to the same λ but to the different m's suggested by the notation.—Thus, if we have one solution, we can use our H operators to go up or down to other solutions; continuing the process we would obtain a ladder of solutions belonging to a fixed λ.

For the proof we multiply (2.2.1a) by ${}^{-}H^{m+1}$ and (2.2.1b) by ${}^{+}H^{m}$. The results are

$$ {}^{-}H^{m+1}\,{}^{+}H^{m+1}({}^{-}H^{m+1}y(\lambda, m)) =[\lambda-L(m+1)]({}^{-}H^{m+1}y(\lambda, m)) \quad (2.2.3a) $$

$$ {}^{+}H^{m}\,{}^{-}H^{m}({}^{+}H^{m}y(\lambda, m)) =[\lambda-L(m)]({}^{+}H^{m}y(\lambda, m)). \quad (2.2.3b) $$

Comparison of (2.2.3a) with (2.2.1b) shows that $y(\lambda, m+1)$ as defined above *is* a solution of our equation with m replaced by $m+1$. Similarly $y(\lambda, m-1)$ is a solution with m replaced by $m-1$.

We can now interpret Eqs. (2.2.1) as stating: going one step up the ladder and one step down (or vice versa) we arrive at the solution from which we started, but multiplied by $\lambda-L(m+1)$ (or $\lambda-L(m)$). Of course, through (2.2.2) we *may* reach a solution which vanishes identically; this important situation, which does not violate Theorem I, will be considered in Theorem IV.

In a restricted sense Eqs. (2.2.2) are equivalent to the original differential equation (2.1.1) or (2.2.1). The restriction turns out to be a fortunate one in that, with the proper interpretation of (2.2.2), it leads us to consider *only* those solutions of (2.1.1) which are quadratically integrable. And, because of the probability interpretation of the wave function in quantum mechanics, we will look for only those solutions which do satisfy this condition. (We have not yet, however, distinguished between those which do and those which do not; our theorem is true in either case.)

2.3 Mutual adjointness of the operators; Theorem II

Theorem II.

$$ \int_a^b \varphi({}^{-}H^{m}f)dx=\int_a^b ({}^{+}H^{m}\varphi)fdx $$

if φf vanishes at the ends of the interval and the integrands are continuous in the interval.—The proof is self-evident.

Our theorem means that the H operators are mutually adjoint.

2.4 Boundary condition; Theorem III

We shall be interested in differential equations whose coefficients have singularities only at the ends of the range of the independent variable. In fact, it will be shown in Sec. 3.1 that the range can be chosen so that this is the case whenever a factorization is possible. The quadratic integrability of a solution will therefore depend entirely on the behavior of the solution near the end points and so the condition of quadratic integrability is essentially a boundary condition. By studying the behavior of the solution and the corresponding H operators near an end point we can establish the following theorem for each of the six general factorization types found in Sec. 3.1:

Theorem III. If $y(\lambda, m)$ is quadratically integrable over the entire range of x and $L(m)$ is an increasing function of m $(0<m)$, then the H operation (2.2.2a) of raising m produces a function which is also quadratically integrable and which vanishes at the end points. If $L(m)$ is a decreasing function of $m(0<m)$ then the H operation (2.2.2b) of lowering m produces a function which is also quadratically integrable and which vanishes at the end points.—The theorem is true under weaker but more complicated conditions but the above result will be sufficient for our purposes. It is *not* true, however, that an H operator never affects integrability; for example, in the terminology introduced later for Class I solutions, a badly behaved $y(\lambda, l+1)$ can be turned into the well-behaved $y(\lambda, l)={}^{+}H^{l+1}y(\lambda, l+1)$.

Theorem III has to be proven for each factorization type, but the proof is much the same in each case.

2.5 Conditions on λ that solutions exist; Theorem IV

We shall divide our problems into two classes:

Class I will be characterized by the fact that $L(m)$ is an increasing function of m. We shall see that this situation usually leads to a finite ladder of solutions belonging to $m=0, 1, 2\cdots l$ for each of a discrete set of values $\lambda_l(l=0, 1, 2\cdots)$ of λ.

Class II solutions will arise when $L(m)$ is a decreasing function of m. We will then usually obtain an infinite ladder of solutions belonging to $m=l, l+1, l+2, \cdots$ for each value $\lambda_l(l=0, 1, 2\cdots)$ of λ.

In each class one end, $y(\lambda_l, l)$, of the ladder can be obtained by a simple quadrature and the other solu-

tions by means of (2.2.2). In those cases where λ is not discrete we still have the recurrence formulas (2.2.2) but have no corresponding starting function $y(\lambda_l, l)$. It is also possible that $L(m)$ be a constant. In this case we again have only the recurrence formulas. Bessel's equation leads to the only important example of this possibility and it is discussed in 5.4.

Theorem IV, which determines λ_l as a function of l, will be proven for problems of Class I. The proof for Class II is essentially the same.

Theorem IV. When $L(m)$ is an increasing function[2] of the integer m for $0<m\leq M$, and $\lambda\leq$ the larger of $L(M)$, $L(M+1)$, then a necessary condition for quadratically integrable solutions is that

$$\lambda=\lambda_l=L(l+1)$$

where l is an integer and $m=0, 1, 2, \cdots l$.—For the proof we assume a "good," that is an integrable, solution $y(\lambda, m)$. Then, because of Theorem III,

$$y(\lambda, m+1)=-H^{m+1}y(\lambda, m)$$

is also a "good" solution, or zero, and vanishes at the end points. We can therefore write

$$\begin{aligned}\int_a^b y^2(\lambda, m+1)dx &= \int_a^b -H^{m+1}y(\lambda, m)\cdot -H^{m+1}y(\lambda, m)dx \\ &= \int_a^b y(\lambda, m)\cdot {}^{+}H^{m+1}\,{}^{-}H^{m+1}y(\lambda, m)dx \quad \text{(Theorem II)} \\ &= [\lambda-L(m+1)]\int_a^b y^2(\lambda, m)dx \qquad \text{(by 2.2.1a)}\end{aligned}$$

where (a, b) is the entire range for x. Similarly:

$$\int_a^b y^2(\lambda, m+2)dx=[\lambda-L(m+2)]\times[\lambda-L(m+1)]\int_a^b y^2(\lambda, m)dx.$$

This argument can be continued and, since $L(m)$ is an increasing function of m, we will arrive at some value of m, say $l+1$, with the contradiction

$$\int_a^b y^2(\lambda, l+1)dx<0$$

unless[3]

$$y(\lambda, l+1)\equiv 0$$

i.e.,
$$-H^{l+1}y(\lambda, l)\equiv 0. \qquad (2.5.1)$$

[2] Usually $M=\infty$ and $L(M)=\infty$.

[3] In case $\lambda>L(M)$ and $L(M+1)$ we are not led to a discrete spectrum for λ. This situation usually corresponds to the unrestricted energy levels of the Kepler problem (see Sec. 7.2 and Chapter 8).

In this case, because of (2.2.1a) we obtain

$$\lambda=\lambda_l=L(l+1).$$

This condition fixes λ in terms of l, one of the possible values of m, the other values of m being less than l. These are, then, the required eigenvalues for λ.

In 2.7 we shall use (2.5.1) along with (2.2.2) to find the eigenfunctions; so far we know only that (2.5.1) is a necessary condition for the existence of Class I eigenfunctions when $\lambda\leq$ the larger of $L(M)$, $L(M+1)$.

The corresponding theorem for Class II solutions states that: *if $L(m)$ is a decreasing function of the integer m for $0\leq m\leq M$ and $\lambda\leq L(0)$, then a necessary condition for the existence of quadratically integrable solutions is that*

$$\lambda=\lambda_l=L(l)$$

where l is an integer and $m=l, l+1, l+2\cdots$.—And, corresponding to (2.5.1), we obtain

$${}^{+}H^{l}y(\lambda, l)\equiv 0.$$

Finally, we should note that, if m_0 of Sec. 2.1 is not taken to be zero, then Theorem IV obviously will require $|l-m|$ rather than l to be an integer.

2.6 *Normalization; Theorem V*

When Theorem III holds we can arrange to have our operators preserve not only the quadratic integrability but the normalization of the eigenfunctions.

We write, instead of (2.2.1),

$${}^{+}\mathfrak{C}_l{}^{m+1}\,{}^{-}\mathfrak{C}_l{}^{m+1}Y_l{}^{m}=Y_l{}^{m}$$

$${}^{-}\mathfrak{C}_l{}^{m}\;{}^{+}\mathfrak{C}_l{}^{m}\;Y_l{}^{m}=Y_l{}^{m}$$

and, instead of (2.2.2),

$$Y_l{}^{m+1}=-\mathfrak{C}_l{}^{m+1}Y_l{}^{m} \qquad (2.6.1a)$$

$$Y_l{}^{m-1}=+\mathfrak{C}_l{}^{m}\;Y_l{}^{m} \qquad (2.6.1b)$$

where

$${}^{\pm}\mathfrak{C}_l{}^{m}=\begin{cases}[L(l+1)-L(m)]^{-\frac{1}{2}}\,{}^{\pm}H^{m} & \text{for Class I problems}\\ [L(l)-L(m)]^{-\frac{1}{2}}\,{}^{\pm}H^{m} & \text{for Class II problems}\end{cases}$$

and where the dependence of the solutions on l rather than λ is suggested by the new notation.

Then, proceeding as in Theorem IV, we obtain

$$\int_a^b (\bar{Y}_l{}^{m+1})^2dx=\int_a^b (Y_l{}^{m})^2dx$$

so that, if $Y_l{}^{l}$ is normalized, so are the other $Y_l{}^{m}$. Hence:

Theorem V.—The $\mathfrak{C}$ operators defined above preserve the normalization of the eigenfunctions, when these functions are normalizable.—Capital letters will be used from now on to represent *normalized* solutions of our equations.

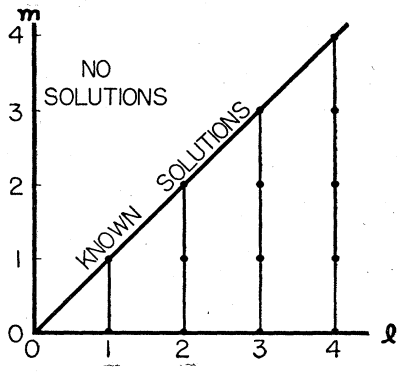


FIG. 1. Each dot represents a Class I solution. The "known solutions" are obtained from (2.7.1); the others from (2.7.2).

2.7 Solutions

We are now able to see how to write down the eigenvalues and normalized eigenfunctions of an equation once that equation has been factorized—i.e., once the $k(x, m)$ and $L(m)$ corresponding to the given $r(x, m)$ are known.

Let us consider in detail the Class I problem. Here $L(m)$ is an increasing function of m and we are only interested in the case when $\lambda \leq$ the larger of $L(M)$, $L(M+1)$.

The eigenvalues, from Theorem IV, are

$$\lambda_l = L(l+1), \quad m=0, 1, 2, \cdots l.$$

Furthermore, Theorem IV tells us that

$$\left\{k(x, l+1)-\frac{d}{dx}\right\}Y_l{}^l=0 \qquad \text{(see 2.5.1)}$$

is a necessary condition for the existence of normalizable eigenfunctions. Therefore

$$Y_l{}^l = C\exp\left(\int k(x, l+1)dx\right) \qquad (2.7.1)$$

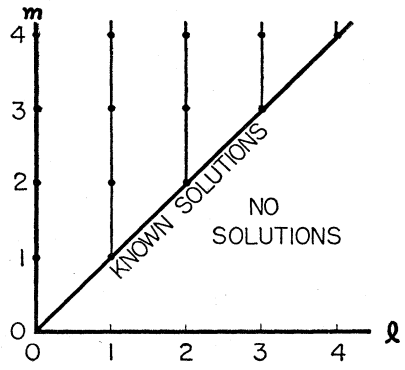


FIG. 2. Each dot represents a Class II solution. The "known solutions" are obtained from (2.7.3); the others from (2.7.4).

where C is a constant to be determined, if possible, by the condition

$$\int_a^b (Y_l{}^l)^2 dx = 1.$$

We must say *if possible* since we do not know in advance that $Y_l{}^l$ is quadratically integrable—we only know that, if it *is*, then (2.7.1) is the correct form. (In most applications we can normalize (2.7.1), but, to do so in some cases, we find it is necessary to further restrict some of the parameters of the problem.)

The other normalized solutions are then given by

$$Y_l{}^{m-1} = +\mathfrak{C}_l{}^m Y_l{}^m = [L(l+1)-L(m)]^{-\frac{1}{2}}\left\{k(x, m)+\frac{d}{dx}\right\}Y_l{}^m. \qquad (2.7.2)$$

Figure 1 represents graphically the usual situation. The solutions of our differential equation (2.1.1) depend on the two parameters l, m; to each pair of values (l, m) there correspond two solutions. If a solution is well-behaved it is represented by a dot in Fig. 1. Only those for which $l \geqslant m$ can satisfy the boundary condition since, only then is $L(l+1)-L(m+1) \geqslant 0$. The solutions along the line $m=l$ are given immediately by a simple quadrature (2.7.1). From each of these a ladder leads down to the other solutions belonging to the same $\lambda = L(l+1)$. They are obtained through (2.7.2).

In Class II problems the usual situation is as shown in Fig. 2. Here $l \leqslant m$ if the solutions are to be well-behaved since only then is $L(l)-L(m) \geqslant 0$. ($L(m)$ is now a *decreasing* function of m.) Now

$$Y_l{}^l = C\exp\left(-\int k(x, l)dx\right) \qquad (2.7.3)$$

where C is a constant to be determined, if possible, by the normalization condition

$$\int_a^b (Y_l{}^l)^2 dx = 1.$$

The other normalized solutions are then given by

$$Y_l{}^{m+1} = -\mathfrak{C}_l{}^{m+1} Y_l{}^m = [L(l)-L(m+1)]^{-\frac{1}{2}}\left\{k(x, m+1)-\frac{d}{dx}\right\}Y_l{}^m. \qquad (2.7.4)$$

Whether we have a problem of Class I or Class II depends on whether $L(m)$ is an increasing or decreasing function of m. Interchanging the roles of l and m in the factorization will change a Class I problem into a Class II problem, or vice versa. That is, a factorization which would provide l-changing recurrence relations in the scheme of Fig. 1 is obviously equivalent to a Class II factorization. The distinction between Classes I and II is therefore not a property of the eigenfunctions,

but rather of the factorization itself. We will find that for the spherical harmonics (Sec. 4.1) it is useful to know *both* factorizations, while for most other problems only *one* factorization is important, namely, the one giving the physically correct normalization.

3. Technique of Factorization

We turn now to the problem of finding a factorization. We want to know what $k(x, m)$, $L(m)$, if any, correspond to a given $r(x, m)$.

In the following section we shall answer the question: "What are all possible types of factorization?" When the six types are exhibited, the problem of factorizing is reduced to that of identifying a given $r(x, m)$ as a special case of one of these six general types.

Section 3.2 completes the technique of factorization by introducing "artificial factorization." This idea usually enables us to solve a problem even when the given $r(x, m)$ differs from one of the possible types in its dependence[4] on m.

3.1 Factorization types

If, in our factorized equations (2.2.1), we carry out the indicated operations and compare with the original equation (2.1.1) we obtain

$$\left.\begin{aligned} k^2(x, m+1)+\frac{dk(x, m+1)}{dx}+L(m+1) &= -r(x, m) \\ k^2(x, m)-\frac{dk(x, m)}{dx}+L(m) &= -r(x, m) \end{aligned}\right\}. \quad (3.1.1)$$

Subtracting we obtain

$$k^2(x, m+1)-k^2(x, m)+\frac{dk}{dx}(x, m+1)+\frac{dk}{dx}(x, m)=L(m)-L(m+1). \quad (3.1.2)$$

This is obviously a necessary condition to be satisfied by $k(x, m)$ and $L(m)$. It is also sufficient since any $k(x, m)$ and $L(m)$ which do satisfy this equation lead unambiguously through (3.1.1) to a function $r(x, m)$ and so to an equation whose factorization is known.

We want to find all $k(x, m)$ and $L(m)$ which will satisfy (3.1.2). First, there is one trivial solution which we will dismiss with only a brief discussion. It is

$$k(x, m)=f(m), \quad L(m)=-f^2(m)$$

where $f(m)$ is any function of m. The differential equation (2.1.1) becomes

$$(d^2y/dx^2)+\lambda y=0.$$

The general solution of this equation is a linear combination of $\sin\lambda^{\frac{1}{2}}x$ and $\cos\lambda^{\frac{1}{2}}x$ and the H operators would merely generate other linear combinations. Schrödinger (42) has given a complete discussion of this problem. He shows how the artificial boundary conditions of a vibrating string problem can, with some patience, be handled by the factorization method; but the method is not suited to such a problem. (The boundary conditions are "artificial" as opposed to the "natural" one of integrability used in quantum mechanics.)

For the more useful solutions of (3.1.2) we begin with the trial solution

$$k(x, m)=k_0+mk_1 \quad (3.1.3)$$

where k_0, k_1 are functions of x only. Substituting into (3.1.2) and letting a prime ($'$) denote differentiation with respect to x we can obtain finally

$$[(m+1)^2(k_1^2+k_1')+2(m+1)(k_0k_1+k_0')]-[m^2(k_1^2+k_1')+2m(k_0k_1+k_0')]=L(m)-L(m+1) \quad (3.1.4)$$

of which the most general solution for $L(m)$ is

$$L(m)=-m^2(k_1^2+k_1')-2m(k_0k_1+k_0')+\tilde{1}$$

where $\tilde{1}$ is a function of m and x of period 1 in m. We are interested only in values of $L(m)$ for integral values of m so we can take

$$\tilde{1}=f(x)$$

where $f(x)$ is an arbitrary function of x. But since the expression for $L(m)$ must hold for all values of m and $L(m)$ is a function of m alone, the coefficients of powers of m on the right side must be separately equal to constants. We can take $f(x)=0$ without loss of generality, and we have

$$k_1^2+k_1'=-a^2 \quad (3.1.5a)$$

$$k_0'+k_0k_1=\left\{\begin{array}{ll} -ca, & \text{if } a\neq 0 \\ b, & \text{if } a=0 \end{array}\right\} \quad (3.1.5b)$$

where a, b, c are constants. These give

$$L(m)=\left\{\begin{array}{ll} a^2m^2+2ca^2m, & \text{if } a\neq 0 \\ -2bm, & \text{if } a=0 \end{array}\right\}. \quad (3.1.6)$$

The solutions of (3.1.5) are (if $a\neq 0$)

(A) $k_1=a\cot a(x+p)$,
$k_0=ca\cot a(x+p)+d/\sin a(x+p)$ (3.1.7a)

[4] Explicit formulas have been given (24) for $k(x, m)$, $L(m)$ in terms of $r(x, m)$. They are

$$k(x, m)=[2r(x, m-1)-2r(x, m)]^{-1}\frac{d}{dx}[r(x, m-1)+r(x, m)]$$

$$L(m)=-[r(x, m-1)+r(x, m)]/2-k^2(x, m).$$

The criterion that a factorization be possible is of course that $L(m)$ be independent of x. These formulas, however, do not admit the possibility of an artificial factorization.

(B) $k_1=ia, \quad k_0=cia+d\exp(-iax)$ (3.1.7b)
or (if $a=0$)

(C) $k_1=1/x, \quad k_0=bx/2+d/x$ (3.1.7c)

(D) $k_1=0, \quad k_0=bx+d$ (3.1.7d)

where d, p are any constants. (We could have written $x+p$ for x in all of these solutions but the generalization is trivial except in (A).)

Our four results are not independent: B, C, D can be considered limiting forms of A. However, the individual forms are each important enough to be exhibited separately.

Each of A to D determines one $k(x, m)$ through (3.1.3) and one $L(m)$ through (3.1.6) which in turn determine one $r(x, m)$ through (3.1.1). These results, along with the other two possible factorizations (which will be found immediately) and many important special cases, are given in the table[5] at the end of this report. They are then ready for the interpretation of Sec. 2.7. The special cases are considered in detail in Chapters 4–8.

It can now be shown that higher powers of m in (3.1.3) lead to nothing new. If we try

$$k(x, m)=k_0+mk_1+m^2k_2$$

we obtain this time, in place of (3.1.4),

$$m^3(4k_2^2)+m^2(6k_2^2+6k_1k_2+2k_2')$$
$$+m(2k_1^2+4k_2^2+4k_0k_2+6k_1k_2+2k_1'+2k_2')$$
$$+\textit{terms not involving } m=L(m)-L(m+1).$$

There is no need to solve for $L(m)$. The coefficients of each power of m on the left side must be constants;

therefore, from the first coefficient: $k_2^2=\text{constant}$
therefore $k_2=\text{constant}$
then, from the second coefficient: $k_1=\text{constant}$, if $k_2\neq 0$
then, from the third coefficient: $k_0=\text{constant}$.

Thus we see that, if $k_2\neq 0$, the only solution is the trivial one discussed at the beginning of this section. No new solutions are obtained through this generalization.

The same argument can be used to show that further generalizations in this direction also produce no new solutions. But the argument breaks down if we allow $k(x, m)$ to have an infinite number of terms in powers of m.

We can, however, find a useful generalization in the other direction. Let us try

$$k(x, m)=k_{-1}/m+k_0+mk_1. \quad (3.1.8)$$

In place of (3.1.4) we obtain

$$-m^2(k_1^2+k_1')-2m(k_0k_1+k_0')-2k_0k_{-1}/m-k_{-1}^2/m^2$$
$$-(\textit{the same expression with } m+1 \textit{ in place of } m)$$
$$+k_{-1}'/m+k_{-1}'/(m+1)=L(m)-L(m+1). \quad (3.1.9)$$

[5] When convenient, we have adjusted $f(x)$ or the constants in the table.

Multiplying (3.1.9) by $m(m+1)^2$ we find the left side becomes a polynomial in m plus one other term:

$$-k_{-1}^2/m.$$

Therefore (3.1.9) can be satisfied only if

$$k_{-1}=q, \text{ say},$$
$$k_{-1}'=0.$$

We do not need to consider $q=0$ since this leads to the cases already discussed. But then, because k_0k_{-1} must be a constant,

$$k_0=\text{constant}.$$

We can omit the case $k_0\neq 0$ for otherwise k_1 would also have to be a constant and we would obtain the "trigonometric" solution again. Therefore we consider only $k_0=0$. In this case the only remaining condition we have is

$$k_1^2+k_1'=-a^2.$$

The constant values of k_1 satisfying this equation lead again to the "trigonometric" solution. We are left with the two new factorization types:

(E) $k_1=a\cot a(x+p), \quad k_0=0, \quad k_{-1}=q$ (3.1.7e)

(F) $k_1=1/x, \quad k_0=0, \quad k_{-1}=q$ (3.1.7f)

and it turns out that

$$L(m)=a^2m^2-q^2/m^2 (a=0 \text{ for } F). \quad (3.1.10)$$

The $k(x, m)$, $L(m)$ and $r(x, m)$ corresponding to types E and F are collected with their special cases in the table and the special cases are discussed in Chapters 7 and 8.

It is a straightforward matter to check that further generalization leads to no new factorizations provided we admit only a finite number of negative powers of m in the expansion of $k(x, m)$.

Of course type F can be considered as a limiting form of type E as $a\to 0$. We therefore have altogether six possible factorization types which are themselves limiting forms of two basic types; we will see later (Chapter 14) that even these two basic types are closely related.

Stevenson (46) was the first to find the above factorization types. He used a different method and found three other types which can, however, be reduced to those considered here.

Finally, it should be noted that, in each of $A-F$, $k(x, m)$, and $r(x, m)$ do in fact have the properties needed to prove Theorem III.

3.2 Artificial factorization

In what follows we shall occasionally have to resort to a device known as artificial factorization. This will be necessary when the given $R(x, m)$ is not quite one of the six basic types. In each case the difference will be in the way the m appears in $R(x, m)$.

There are three possibilities which may appear together but which we will treat separately. For definiteness we will consider only a Class I problem.

The first possibility is that the given $R(x, m)$ is

$$R(x, m)=r(x, m)+f(m)$$

where $r(x, m)$ is one of the standard types and $f(m)$ is an arbitrary function of m. To handle such an example we define

$$\lambda'=\lambda+f(m)$$

and then proceed to solve the new equation

$$(d^2y/dx^2)+r(x, m)y+\lambda'y=0.$$

For normalizable solutions $\lambda'=L(l+1)$ and we can move down a ladder to the solution Y_l^m which belongs to the eigenvalue $\lambda=L(l+1)-f(m)$. In effect the λ (but not λ') changes as we go down the ladder.

The second possibility is that we can introduce a new function $r(x, m, \mu)$ which is a standard type (if we consider μ just a parameter) but such that

$$r(x, m, m)=R(x, m).$$

We can then solve the equation

$$(d^2y/dx^2)+r(x, m, \mu)y+\lambda y=0$$

and obtain a solution $Y_l^m(\mu)$ depending on the parameter μ as well as m and $\lambda=L(l+1)$. The required solution is then merely $Y_l^m(m)$. Part of the dependence of this solution on m has been provided by the ladder operators while the remainder of this dependence has been introduced at the end of the ladder operations by putting $\mu=m$.

The third possibility is that

$$R(x, m)=R(x)=r(x, m) \text{ for } m=p$$

so that the required solution is that of the more general equation (with $r(x, m)$) for the special value p of m.

Even if a *direct* factorization is not possible there may still be an *artificial* factorization and the finding of this artificial factorization is now an explicit procedure: the list of types is consulted for one in which the dependence of $r(x, m)$ on x is the same as that in the given $R(x, m)$. The dependence on m can then *usually* be adjusted by means of the above methods so that a factorization is achieved and the solutions can be found.

4. Type *A* Factorizations and General Remarks

Before presenting the first general factorization type we would like to make a few remarks concerning all types of factorizations.

Each type includes a number of special cases which are obtained merely by an appropriate choice of the parameters appearing in the general type; we will exhibit those which most frequently occur in physics and show, in each case, how the solution of the problem can be obtained readily by the factorization method.

Where necessary we shall give a reference to discussion of the physical interpretation of our results; in some cases it will be found that the problem was first solved by the factorization method.

We want to present our results in the form most useful to physicists. Consequently our notation will differ from that of the general discussion of the previous sections when we are dealing with familiar problems. For the same reason we shall arrange that the normalization preserved by the hypergeometric function operators (in 4.8) differs from that of other examples; we have in mind applications to the calculation of intensities in a later section (12.5) for which it seems preferable to use the usual definition of these functions.

The table at the end of this report collects the $r(x, m)$ and corresponding $k(x, m)$, $L(m)$ functions. The difficulty of solving an eigenvalue problem is then reduced to that of finding the appropriate $r(x, m)$ in the table and using the corresponding $k(x, m)$, $L(m)$ to write down the eigenvalues and normalized eigenfunctions as shown in Chapter 2. The table also includes references to the text where these solutions are given for the more important examples.

From (3.1.1), (3.1.3), (3.1.6), and (3.1.7a) we obtain the first general factorization type. Corresponding to

$$r(x, m)=-\frac{a^2(m+c)(m+c+1)+d^2+2ad(m+c+\frac{1}{2})\cos a(x+p)}{\sin^2 a(x+p)} \tag{4.0.1}$$

the factorization is given by

$$\left.\begin{aligned} k(x, m)&=(m+c)a\cot a(x+p)+d/\sin a(x+p)\\ L(m)&=a^2(m+c)^2\end{aligned}\right\} \tag{4.0.2}$$

where a, c, d, p are constants. For convenience we have chosen a^2c^2 rather than 0 for the $\tilde{1}=f(x)$ of Sec. 3.1.

The results of Sec. 2.7 could now be used to write down the eigenvalues and normalized eigenfunctions of the corresponding differential equation; but, since these results depend on whether $L(m)$ is an increasing or a decreasing function of m and hence on whether a is real or pure imaginary, we will give the solutions for special cases only. At the same time these solutions will appear in readily usable forms.

Our first example will be treated in somewhat greater detail than later ones.

4.1 Associated spherical harmonics

The differential equation satisfied by the associated spherical harmonics is

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)-\frac{m^2}{\sin^2\theta}P+\lambda P=0 \qquad (4.1.1)$$

where $m=0, 1, 2, \cdots$ and $0\leq\theta\leq\pi$.

We bring this equation to the standard form by means of the substitution (Sec. 2.1)

$$Y=\sin^{\frac{1}{2}}\theta P. \qquad (4.1.2)$$

Thus, Y is the density function belonging to the associated spherical harmonic P. Equation (4.1.1) becomes

$$\frac{d^2Y}{d\theta^2}-\frac{m^2-\frac{1}{4}}{\sin^2\theta}Y+(\lambda+\tfrac{1}{4})Y=0. \qquad (4.1.3)$$

But the potential function here is exactly our type A (4.0.1) if we put in the latter

$$a=1, \quad c=-\tfrac{1}{2}, \quad d=0, \quad p=0, \quad x=\theta$$

and replace λ by $\lambda+\frac{1}{4}$. Therefore the factorization is given by

$$k(\theta, m)=(m-\tfrac{1}{2})\cot\theta$$
$$L(m)=(m-\tfrac{1}{2})^2.$$

$L(m)$ is an increasing function of m. We therefore have a Class I problem and the eigenvalues must be

$$\lambda+\tfrac{1}{4}=L(l+1)$$

so that

$$\lambda=l(l+1)$$

where $l=0, 1, 2\cdots$ and $l\geq m$ and the corresponding normalized solutions are given by

$$Y_l^l=\left[\frac{1\cdot3\cdot5\cdot\cdots 2l+1}{2\cdot2\cdot4\cdot\cdots 2l}\right]^{\frac{1}{2}}\sin^{l+\frac{1}{2}}\theta \qquad (4.1.4a)$$

and

$$Y_l^{m-1}=[(l+m)(l+1-m)]^{-\frac{1}{2}}\times\left\{(m-\tfrac{1}{2})\cot\theta+\frac{d}{d\theta}\right\}Y_l^m. \qquad (4.1.4b)$$

Equations (4.1.4) define the eigenfunctions of Legendre's equation. We shall show later that this way of expressing the result is not only quickly obtained by the factorization method but is also in a very convenient form; for one thing, the physically proper normalization is preserved.

We shall also need later the m-raising recurrence relation[6]

$$Y_l^{m+1}=[(l+m+1)(l-m)]^{-\frac{1}{2}}\times\left\{(m+\tfrac{1}{2})\cot\theta-\frac{d}{d\theta}\right\}Y_l^m. \qquad (4.1.4c)$$

Of course we did not know in advance that Y_l^l would satisfy the boundary conditions. However, once Y_l^l is found, we see immediately that all the functions Y_l^m *do* satisfy the boundary conditions. If Y_l^l had not, then we would know from the general theory that there were no normalizable eigenfunctions at all.

For negative m it is seen from (4.1.3) that

$$Y_l^{-m}=\pm Y_l^m.$$

A study of the nature of the ladder operations near $m=0$ will reveal that the operators can be used to reach the eigenfunctions for negative values of m. The result of going down the ladders to these values of m turns out to be

$$Y_l^{-m}=(-1)^m Y_l^m.$$

4.2 Associated spherical harmonics as a Class II problem

If we introduce $l(l+1)$ for λ and replace $-m^2$ by λ, Eq. (4.1.1) becomes

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)+l(l+1)P+\frac{\lambda}{\sin^2\theta}P=0, \quad l=0, 1, 2\cdots.$$

Let us now consider the possibility of finding a factorization of this equation which will enable us to raise and lower the l parameter while keeping the new λ fixed. The normal form *now* is obtained by putting

$$z=\log\tan(\theta/2). \qquad (4.2.1)$$

Let us also write $\bar{P}$ for P and reserve the symbol P for the properly normalized solutions. Our equation becomes

$$\frac{d^2\bar{P}}{dz^2}+\frac{l(l+1)}{\cosh^2 z}\bar{P}+\lambda\bar{P}=0 \qquad (4.2.2)$$

which is type A (4.0.1) again but with $a=i$, $c=0$, $p=i\pi/2$, $d=0$, and with x, m replaced z, l. The factorization is therefore given by

$$k(z, l)=l\tanh z$$
$$L(l)=-l^2.$$

Since $L(l)$ is a decreasing function of l we have a Class II factorization and the bottom of the ladder is ob-

[6] The operators in (4.1.4) are closely related to orbital angular momentum operators. If L_x, L_y are the first two components of the orbital angular momentum, then (37, p. 439):

$$L_x\pm iL_y=\hbar\exp(\pm i\varphi)\left(\pm\frac{\delta}{\delta\theta}+i\cot\theta\frac{\delta}{\delta\varphi}\right).$$

tained by taking λ such that $\lambda=-l^2$ for some value of l, say, m. Therefore, $\lambda=-m^2$ where $l-m=0, 1, 2, \cdots$.

The corresponding ladder of normalized solutions satisfying the boundary condition (quadratic integrability over the interval $-\infty, \infty$) is

$$\bar{P}_m{}^m, \bar{P}_{m+1}{}^m, \bar{P}_{m+2}{}^m, \cdots \bar{P}_l{}^m, \cdots$$

where

$$\bar{P}_m{}^m=\left(\frac{1\cdot 3\cdot 5\cdot \cdots \cdot 2m-1}{2\cdot 2\cdot 4\cdot \cdots \cdot 2m-1}\right)^{\frac{1}{2}} \cosh^{-m}z \tag{4.2.3a}$$

$$\bar{P}_l{}^m=[(l-m)(l+m)]^{-\frac{1}{2}}\left\{l \tanh z-\frac{d}{dz}\right\}\bar{P}_{l-1}{}^m. \tag{4.2.3b}$$

Because of (4.2.1) we can write for future reference

$$\left\{-l\cos\theta-\sin\theta\frac{d}{d\theta}\right\}\bar{P}_{l-1}{}^m =[(l-m)(l+m)]^{\frac{1}{2}}\bar{P}_l{}^m \tag{4.2.4a}$$

$$\left\{-l\cos\theta+\sin\theta\frac{d}{d\theta}\right\}\bar{P}_l{}^m =[(l-m)(l+m)]^{\frac{1}{2}}\bar{P}_{l-1}{}^m. \tag{4.2.4b}$$

There are important differences between $\bar{P}$ and Y. $\bar{P}$ can be written as a function of θ and then

$$Y\sim\sin^{\frac{1}{2}}\theta\bar{P}\equiv\bar{Y}, \quad \text{say.}$$

The other important difference is in the normalization. Y is normalized so that

$$\int_0^\pi Y^2 d\theta=1 \tag{4.2.5}$$

while

$$\int_{-\infty}^{\infty}\bar{P}^2dz=1$$

which would correspond to

$$\int_0^\pi(\bar{Y}^2/\sin^2\theta)d\theta=1.$$

In the calculation of the spherical harmonic matrix elements (Sec. 9.1) we shall see how the connection between these two normalizations is to be found. In physical applications it is the normalization of Y which corresponds to the probability interpretation of the wave functions. Therefore, it is desirable to adjust the constants in (4.2.4) so that the Y, rather than the $\bar{P}$ (or $\bar{Y}$), normalization is preserved.

4.3 Generalized spherical harmonics

The generalized spherical harmonics satisfy

$$\frac{d^2\Phi}{d\theta^2}+2\gamma\cot\theta\frac{d\Phi}{d\theta}-\frac{m^2+2m\gamma-m}{\sin^2\theta}\Phi+\lambda\Phi=0$$

where m is, as before, a non-negative interger and γ is an arbitrary positive parameter. This equation takes the standard form

$$\frac{d^2Y}{d\theta^2}-\frac{(m+\gamma)(m+\gamma-1)}{\sin^2\theta}Y+(\lambda+\gamma^2)Y=0 \tag{4.3.1}$$

through the substitution

$$Y=\sin^\gamma\theta\Phi.$$

Using type A with $a=1$, $c=\gamma-1$, $d=p=0$ we obtain the Class I solutions:

$$\lambda=l(l+2\gamma)$$

$$Y_{l,\gamma}{}^l=\pi^{-\frac{1}{4}}\left[\frac{\Gamma(l+\gamma+1)}{\Gamma(l+\gamma+\frac{1}{2})}\right]^{\frac{1}{2}}\sin^{l+\gamma}\theta$$

$$Y_{l,\gamma}{}^{m-1}=[(l+m+2\gamma-1)(l-m+1)]^{-\frac{1}{2}} \times\left\{(m+\gamma-1)\cot\theta+\frac{d}{d\theta}\right\}Y_{l,\gamma}{}^m$$

where m cannot be $\leq-\gamma-\frac{1}{2}$ unless $\gamma=\frac{1}{2}$. (The solutions for negative m can be obtained from

$$Y_{l,\gamma}{}^{-m}=Y_{l,\gamma}{}^{m+1} \quad \text{when} \quad \lambda=l(l-2\gamma).)$$

These results reduce to those of Sec. 4.1 for $\gamma=\frac{1}{2}$. For $\gamma=1$ we obtain the radial functions for a free particle in a spherical space which is also a special case of the problem treated in Sec. 7.1.

The Class II problem (see 4.2) is obtained through the substitutions

$$\lambda=l(l+2\gamma)$$
$$z=\log\tan(\theta/2)$$
$$\bar{P}\sim\sin^{\gamma-\frac{1}{2}}\theta\Phi$$

giving

$$\frac{d^2\bar{P}}{dz^2}+\frac{(l+\gamma-\frac{1}{2})(l+\gamma+\frac{1}{2})}{\cosh^2z}\bar{P} -[(\gamma-\tfrac{1}{2})^2+2m\gamma+m^2-m]\bar{P}=0. \tag{4.3.2}$$

The solutions are

$$\bar{P}_{m,\gamma}{}^m=\pi^{-\frac{1}{4}}\left[\frac{\Gamma(m+\gamma)}{\Gamma(m+\gamma-\frac{1}{2})}\right]^{\frac{1}{2}}\cosh^{-m-\gamma+\frac{1}{2}}z$$

$$\bar{P}_{l,\gamma}{}^m=[(l-m)(l+m+2\gamma-1)]^{-\frac{1}{2}} \times\left\{(l+\gamma-\tfrac{1}{2})\tanh z-\frac{d}{dz}\right\}\bar{P}_{l-1,\gamma}{}^m.$$

The differences between $\bar{P}_{l,\gamma}{}^m$ and $Y_{l,\gamma}{}^m$ are important and completely analogous to those between $\bar{P}$ and Y of the two preceding sections.

4.4 Gegenbauer functions

The Gegenbauer functions can be defined through the differential equation (53, p. 329)

$$(1-z^2)\frac{d^2U}{dz^2}-(2m+3)z\frac{dU}{dz}+\lambda U=0.$$

If we put

$$z=-\cos\theta$$
$$U=Y\sin^{-m-1}\theta$$

we obtain the standard form,

$$\frac{d^2Y}{d\theta^2}-\frac{m(m+1)}{\sin^2\theta}Y+(\lambda+(m+1)^2)Y=0. \quad (4.4.1)$$

Now we have a type A equation except that we have to proceed as explained in Sec. 3.2 and introduce the artificial

$$\lambda'=\lambda+(m+1)^2$$

the factorization is then given by

$$k(\theta, m)=m\cot\theta$$
$$L(m)=m^2$$

and the solutions are defined by

$$Y_l{}^l=\pi^{-\frac{1}{2}}\left[\frac{\Gamma(l+2)}{\Gamma(l+\frac{3}{2})}\right]^{\frac{1}{2}}\sin^{l+1}\theta$$

$$Y_l{}^{m-1}=[(l+1-m)(l+1+m)]^{-\frac{1}{2}}\left\{m\cot\theta+\frac{d}{d\theta}\right\}Y_l{}^m;$$

also $Y_l{}^{-m}=Y_l{}^{m-1}$ after putting $\lambda'=\lambda+(m-1)^2$.

We should emphasize the fact that $Y_l{}^m$ belongs to the eigenvalue

$$\lambda'=(l+1)^2, \quad l-m=0, 1, 2, \cdots$$

that is, to

$$\lambda=(l-m)(l+m+2).$$

4.5 Symmetric top

The wave equation for a symmetric top is important in the study of simple molecules. Following Dennison (7, p. 310), the wave function is

$$U=\Theta(\theta)\exp(iK\varphi)\exp(iM\psi)$$

where θ, φ, ψ are Eulerian angles and K, M are integers. The first part of this function satisfies

$$\frac{d^2\Theta}{d\theta^2}+\cot\theta\frac{d\Theta}{d\theta}-\frac{(M-K\cos\theta)^2}{\sin^2\theta}\Theta+\sigma\Theta=0$$

and

$$\sigma=8\pi^2AW/h^2-AK^2/C.$$

If we make the substitution

$$Y=\sin^{\frac{1}{2}}\theta\Theta$$

we obtain

$$\frac{d^2Y}{d\theta^2}-\left[\frac{(M-\frac{1}{2})(M+\frac{1}{2})+K^2-2MK\cos\theta}{\sin^2\theta}\right]Y$$
$$+(\sigma+K^2+\tfrac{1}{4})Y=0 \quad (4.5.1)$$

which can be identified with type A if in the latter we put $a=1$, $c=-\frac{1}{2}$, $d=-K$, $p=0$. The factorization is given by

$$k(\theta, M)=(M-\tfrac{1}{2})\cot\theta-\frac{K}{\sin\theta}$$
$$L(M)=(M-\tfrac{1}{2})^2.$$

The solutions are therefore

$$Y_{J,K}{}^J=\left[\frac{\Gamma(2J+2)}{\Gamma(J-K+1)\Gamma(J+K+1)}\right]^{\frac{1}{2}}$$
$$\times\sin^{J-K+\frac{1}{2}}\frac{\theta}{2}\cos^{J+K+\frac{1}{2}}\frac{\theta}{2}$$
$$Y_{J,K}{}^{M-1}=[(J+M)(J-M+1)]^{-\frac{1}{2}}$$
$$\times\left\{(M-\tfrac{1}{2})\cot\theta-\frac{K}{\sin\theta}+\frac{d}{d\theta}\right\}Y_{J,K}{}^M$$

corresponding to the eigenvalues

$$\sigma+K+\tfrac{1}{4}=(J+\tfrac{1}{2})^2, \quad J-|M|, \quad J-|K|=0, 1, 2, \cdots$$

so that

$$W=\frac{J(J+1)h^2}{8\pi^2A}+\left(\frac{1}{C}-\frac{1}{A}\right)\frac{K^2h^2}{8\pi^2}.$$

4.6 Weyl's spherical harmonics with spin

Schrödinger's quantum-mechanical theory leads to one amplitude equation of the second order. Dirac's theory accounts for the spin and leads instead to pairs of first-order equations for the spin components of the eigenfunctions. In this section and in 8.4 we will treat such a pair of equations *directly* by the factorization method. The idea is to transform these equations so that they are *themselves* a factorization.

After separating variables Weyl (51, p. 230) obtains the following equations for the dependence of the components of the wave function on the azimuth angle:

$$\left.\begin{aligned}\sin\theta\frac{df}{d\theta}-mf+k(1+\cos\theta)g=0\\ \sin\theta\frac{dg}{d\theta}+mg-k(1-\cos\theta)f=0\end{aligned}\right\} \quad (4.6.1)$$

where m is a given integer and k is to be found.

Now it is easy to see that, if we introduce

$$\left.\begin{aligned} P_1 &= g+f \\ P_2 &= g-f \end{aligned}\right\} \tag{4.6.2}$$

and add and subtract Eqs. (4.6.1) in turn, we obtain

$$\left(-k\cos\theta-\sin\theta\frac{d}{d\theta}\right)P_1=(k+m)P_2$$

$$\left(-k\cos\theta+\sin\theta\frac{d}{d\theta}\right)P_2=(k-m)P_1.$$

But these are exactly Eqs. (4.2.4) if we identify

$$P_1=2C(k+m)^{\frac{1}{2}}\bar{P}_{k-1}{}^m$$

$$P_2=2C(k-m)^{\frac{1}{2}}\bar{P}_k{}^m$$

where C is a constant which depends on the normalization. The required solutions are therefore (see 42)

$$f=C\{(k+m)^{\frac{1}{2}}\bar{P}_{k-1}{}^m-(k-m)^{\frac{1}{2}}\bar{P}_k{}^m\}$$

$$g=C\{(k+m)^{\frac{1}{2}}\bar{P}_{k-1}{}^m+(k-m)^{\frac{1}{2}}\bar{P}_k{}^m\}$$

and k must be an integer not less than m.

We have considered only positive m but, of course,

$$\bar{P}_k{}^m=(-1)^m\bar{P}_k{}^m, \quad P_1(k)=P_2(-k).$$

A second method of solution is obtained by introducing

$$F=\tan(\theta/2)f, \quad G=\tan(\theta/2)g \tag{4.6.3}$$

so that (4.6.1) becomes

$$\left.\begin{aligned} \left\{\frac{m+\frac{1}{2}}{\sin\theta}-\frac{d}{d\theta}\right\}F &= kG \\ \left\{\frac{m+\frac{1}{2}}{\sin\theta}+\frac{d}{d\theta}\right\}G &= kF; \end{aligned}\right\} \tag{4.6.4}$$

then

$$\frac{d^2F}{d\theta^2}-\frac{m(m+1)+\frac{1}{4}-(m+\frac{1}{2})\cos\theta}{\sin^2\theta}F+k^2F=0 \tag{4.6.5a}$$

$$\frac{d^2G}{d\theta^2}-\frac{m(m+1)+\frac{1}{4}+(m+\frac{1}{2})\cos\theta}{\sin^2\theta}G+k^2G=0. \tag{4.6.5b}$$

But these are type A equations with $a=1$, $c=p=0$, $d=\mp\frac{1}{2}$ respectively. The solutions for $k^2=(l+1)^2$ are

$$\left.\begin{matrix} F_l{}^l \\ G_l{}^l \end{matrix}\right\}=\left[\frac{\Gamma(2l+3)}{\Gamma(l+1)\Gamma(l+2)}\right]^{\frac{1}{2}}\left\{\begin{matrix} \sin^{l+\frac{1}{2}}(\theta/2)\cos^{l+\frac{3}{2}}(\theta/2) \\ \sin^{l+\frac{3}{2}}(\theta/2)\cos^{l+\frac{1}{2}}(\theta/2) \end{matrix}\right\}$$

$$\left.\begin{matrix} F_l{}^{m-1} \\ G_l{}^{m-1} \end{matrix}\right\}=[(l-m+1)(l+m+1)]^{-\frac{1}{2}}\left\{m\cot\theta\mp\frac{1}{2\sin\theta}+\frac{d}{d\theta}\right\}\left\{\begin{matrix} F_l{}^m \\ G_l{}^m \end{matrix}\right\}. \tag{4.6.6}$$

Using (4.6.3) we can obtain f, g; and of course

$$F_k{}^{-m}=G_k{}^{m-1}, \quad G_k{}^{-m}=-F_k{}^{m-1},$$

$$F_{-k}{}^m=F_k{}^m, \quad G_{-k}{}^m=-G_k{}^m.$$

4.7 *Magnetic pole equation*

Dirac (8) first introduced the wave equation for an electron moving in the field of a fixed magnetic pole. After separating variables he obtains the following equation:

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left[\sin\theta\frac{d}{d\theta}S\right]-\left[\frac{m^2}{\sin^2\theta}+\frac{1}{2}m\sec^2\frac{\theta}{2}+\frac{1}{4}\tan^2\frac{\theta}{2}\right]S+\lambda S=0$$

where m is an integer and λ is to be found. Putting

$$T=\sin^{\frac{1}{2}}\theta S$$

we obtain

$$\frac{d^2T}{d\theta^2}-\left[\frac{m(m+1)+\frac{1}{4}-(m+\frac{1}{2})\cos\theta}{\sin^2\theta}\right]T$$

$$+(\lambda+\tfrac{1}{2})T=0 \tag{4.7.1}$$

which is type A with $a=1$, $c=p=0$, $d=-\frac{1}{2}$, and λ replaced by $\lambda+\frac{1}{2}$ so that the eigenvalues are

$$\lambda=L(l+1)-\tfrac{1}{2}$$
$$=l^2+2l+\tfrac{1}{2}, \quad l=0, 1, 2, \cdots$$

which agrees with the result given by Tamm (48).

The solutions are exactly (4.6.6) for F.

4.8 *Pöschl-Teller potentials*

In a later section (5.2) we shall consider the potential function which was suggested by Morse to explain the observed vibrational energy levels and dissociation energies of diatomic molecules. There have since been proposed other potential functions which lead to the same energy eigenvalues but which involve more than the two parameters of the Morse potential and which can therefore be adjusted to fit more spectroscopic data. Two of these functions were given by Pöschl and Teller and we shall now show that they are each special cases of our type A problem so that we shall be able to write down the solutions immediately. In fact we should look upon a familiarity with type A (and later type B) as enabling us to *discover* such potential functions.

The first Pöschl-Teller equation is (36)

$$\frac{d^2\psi}{dr^2}-\left[\frac{\alpha^2\nu(\nu-1)}{\sin^2\alpha(r-r_0)}+\frac{\alpha^2\mu(\mu-1)}{\cos^2\alpha(r-r_0)}\right]\psi+\frac{8\pi^2M}{h^2}E\psi=0.$$

By putting $a=2\alpha$, $c=0$, $d=2g\alpha$, $x=r$, $p=-r_0$ the potential function of type A becomes

$$-\frac{\alpha^2(m+g)(m+g+1)}{\sin^2\alpha(r-r_0)}-\frac{\alpha^2(m-g)(m-g+1)}{\cos^2\alpha(r-r_0)} \quad (4.8.1)$$

and we can identify $m+g+1$, $m-g+1$ with ν, μ respectively so that $2m+2=\mu+\nu$.

The factorization is given by

$$k(r, m)=(m+g)\alpha\cot\alpha(r-r_0)-(m-g)\alpha\tan\alpha(r-r_0)$$
$$L(m)=4\alpha^2m^2$$

which is therefore a Class I problem so that the eigenvalues are

$$\lambda=4\alpha^2(l+1)^2, \quad l=m+n, \quad n=0, 1, 2, \cdots$$

that is,

$$E_n=\frac{\alpha^2h^2}{8\pi^2M}(\mu+\nu+2n)^2, \quad n=0, 1, 2, \cdots$$

as given by Pöschl and Teller.

The normalized eigenfunctions are obtained through

$$\psi_n=\psi_{m+n}{}^m$$

where

$$\psi_l{}^l=\left[\frac{2\alpha\Gamma(2l+3)}{\Gamma(l+\frac{3}{2}+g)\Gamma(l+\frac{3}{2}-g)}\right]^{\frac{1}{2}}\times\sin^{l+1+g}\alpha(r-r_0)\cos^{l+1-g}\alpha(r-r_0)$$

$$\psi_l{}^m=\frac{1}{2\alpha}[(l+2+m)(l-m)]^{-\frac{1}{2}}\left\{k(r, m+1)+\frac{d}{dr}\right\}\psi_l{}^{m+1}$$

provided $m+\frac{3}{2}>|g|$.

We have introduced the n because, from the physical point of view, we consider the m in the potential function as a given constant and we look for eigenfunctions belonging to different l (or n). The eigenfunctions occupy one *row* in Fig. 1 and are numbered from left to right by $n=0, 1, 2, \cdots$. (We recall that m, l themselves need not be integers as long as their difference n is an integer.)

The second Pöschl-Teller equation is

$$\frac{d^2\psi}{dr^2}-\left[\frac{\alpha^2\nu(\nu-1)}{\sinh^2\alpha(r-r_0)}-\frac{\alpha^2\mu(\mu+1)}{\cosh^2\alpha(r-r_0)}\right]\psi+\frac{8\pi^2M}{h^2}E\psi=0.$$

Putting $a=2i\alpha$, $c=0$, $d=2ig\alpha$, $x=r$, $p=-r_0$ we find the potential function of type A becomes

$$-\left[\frac{\alpha^2(m+g)(m+g+1)}{\sinh^2\alpha(r-r_0)}-\frac{\alpha^2(m-g)(m-g+1)}{\cosh^2\alpha(r-r_0)}\right] \quad (4.8.2)$$

and we can identify $m+g$, $m-g$ with $-\nu$, μ respectively so that $2m=\mu-\nu$.

The factorization becomes

$$k(r, m)=(m+g)\alpha\coth\alpha(r-r_0)+(m-g)\alpha\tanh\alpha(r-r_0)$$
$$L(m)=-4\alpha^2m^2$$

which is a Class II problem so that

$$\lambda=-4\alpha^2l^2, \quad l=m-n, \quad n=0, 1, 2, \cdots<m.$$

This time, for a fixed m, there are only a finite number of eigenvalues

$$E_n=\frac{-\alpha^2h^2}{8\pi^2M}(\mu-\nu-2n)^2, \quad n=0, 1, 2, \cdots<(\mu-\nu)/2,$$

and the solutions are

$$\psi_n=\psi_{m-n}{}^m$$

where

$$\psi_l{}^l=\left[\frac{2\alpha\Gamma(l-g+\frac{1}{2})}{\Gamma(-l-g+\frac{1}{2})\Gamma(2l)}\right]^{\frac{1}{2}}\times\sinh^{-l-g}\alpha(r-r_0)\cosh^{-l+g}\alpha(r-r_0)$$

$$\psi_l{}^m=\frac{1}{2\alpha}[(m+l)(m-l)]^{-\frac{1}{2}}\left\{k(r, m)-\frac{d}{dr}\right\}\psi_l{}^{m-1}$$

provided $g<\frac{1}{2}-m$, i.e., $\nu>-\frac{1}{2}$.

4.9 Hypergeometric functions

The differential equation satisfied by the hypergeometric function $F(a, b, c, z)$ is (53, p. 283).

$$z(1-z)\frac{d^2F}{dz^2}+\{c-(a+b+1)z\}\frac{dF}{dz}-abF=0. \quad (4.9.1)$$

We whall factorize this equation in four different ways. However, the results will turn out to be essentially those of the previous section. We shall therefore use our factorizations only to develop certain recurrence relations which we need for the calculation of Dirac matrix elements in Sec. 12.5.

Equation (4.9.1) can be put into the standard form by means of the substitution

$$z=\sin^2\rho$$
$$F=\sin^{-c+\frac{1}{2}}\rho\cos^{-a-b+c-\frac{1}{2}}\rho V.$$

We obtain

$$\frac{d^2V}{d\rho^2}-\frac{(c-\frac{3}{2})(c-\frac{1}{2})}{\sin^2\rho}V-\frac{(a+b-c-\frac{1}{2})(a+b-c+\frac{1}{2})}{\cos^2\rho}V+(a-b)^2V=0. \quad (4.9.2)$$

If we now introduce

$$\frac{d^2V}{d\rho^2}-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sin^2\rho}V - \frac{(m+a+b-c-\frac{1}{2})(m+a+b-c+\frac{1}{2})}{\cos^2\rho}V + (a-b)^2V=0 \quad (4.9.3)$$

the problem becomes that of Sec. 4.8 with the factorization given by

$$k(\rho, m)=(m+c-\tfrac{3}{2})\cot\rho-(m+a+b-c-\tfrac{1}{2})\tan\rho$$
$$L(m)=(2m+a+b-2)^2.$$

Here raising m by 1 corresponds to raising each of a, b, c by 1.

But we can also introduce

$$\frac{d^2V}{d\rho^2}-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sin^2\rho}V - \frac{(m+c-a-b-\frac{1}{2})(m+c-a-b+\frac{1}{2})}{\cos^2\rho}V + (a-b)^2V=0 \quad (4.9.4)$$

with the factorization

$$k(\rho, m)=(m+c-\tfrac{3}{2})\cot\rho-(m+c-a-b-\tfrac{1}{2})\tan\rho$$
$$L(m)=(2m+2c-a-b-2)^2$$

which leads to recurrence formulas for raising and lowering c by unity. This factorization is equivalent to Schrödinger's (43).

If we now consider $(c-1)^2$ in the second term of (4.9.2) as the λ-term to be held constant on the ladders, the standard form will be obtained through

$$V=\sin^{\frac{1}{2}}\rho\, U$$
$$\rho=2\tan^{-1}\exp(-y).$$

We obtain

$$\frac{d^2U}{dy^2}-\frac{(m+a+b-c-\frac{1}{2})(m+a+b-c+\frac{1}{2})}{\sinh^2 y}U + \frac{(m+a-b-\frac{1}{2})(m+a-b+\frac{1}{2})}{\cosh^2 y}U - (c-1)^2U=0 \quad (4.9.5)$$

where m has been introduced as above. Again, as in Sec. 4.8,

$$k(y, m)=(m+a+b-c-\tfrac{1}{2})\coth y+(m+a-b-\tfrac{1}{2})\tanh y$$
$$L(m)=-(2m+2a-c-1)^2$$

and this factorization leads to a-changing recurrence formulas.

Finally another standard form is obtained if we think of the $(a+b-c)^2$ in the third term of (4.9.2) as being the λ to be held constant. The substitution is

$$V=\cos^{\frac{1}{2}}\rho\, W$$
$$\rho=\sin^{-1}(\tanh x)$$

and the resulting equation (with m inserted) is

$$\frac{d^2W}{dx^2}-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sinh^2 x}W + \frac{(m+a-b-\frac{1}{2})(m+a-b+\frac{1}{2})}{\cosh^2 x}W - (a+b-c)^2W=0 \quad (4.9.6)$$

and the a- and c-changing factorization is given by

$$k(x, m)=(m+c-\tfrac{3}{2})\coth x+(m+a-b-\tfrac{1}{2})\tanh x$$
$$L(m)=-(2m+a+c-b-2)^2.$$

The a-changing and c-changing operators can be written in terms of the variables F and z. At the same time the normalization factor can be adjusted so that the constant term in the series for F is unity. The following recurrence formulas are obtained, after putting $m=0$:

$$\left.\begin{aligned}
F(a+1, b, c, z)&=\left\{1+\frac{z}{a}\frac{d}{dz}\right\}F(a, b, c, z) && a\neq 0\\
F(a-1, b, c, z)&=\left\{1+\frac{bz}{a-c}-\frac{z(1-z)}{a-c}\frac{d}{dz}\right\}F(a, b, c, z) && a\neq c\\
F(a, b, c+1, z)&=\frac{c}{(b-c)(c-a)}\left\{a+b-c-(1-z)\frac{d}{dz}\right\}F(a, b, c, z) && \begin{matrix}a\neq c\\ b\neq c\end{matrix}\\
F(a, b, c-1, z)&=\left\{1+\frac{z}{c-1}\frac{d}{dz}\right\}F(a, b, c, z) && c\neq 1
\end{aligned}\right\}. \quad (4.9.7)$$

There are, of course, other first-order differential-difference relations but the above are basic in that any others can be constructed from them. This is true because, as long as the restrictions noted in (4.9.7) are not violated, we can find a product of operators which will turn $F(a, b, c, z)$ into $F(a+\alpha, b+\beta, c+\gamma, z)$ where α, β, γ are integers; and this product can be written as a single first-order operator by expanding, and using the original Eq. (4.9.1) to convert second derivative operators, as they appear, into first-order operators.

Furthermore, it follows that a *sum* of hypergeometric functions contiguous to $F(a, b, c, z)$ can, if the restrictions are not violated, be written in the form $0F(a, b, c, z)$ where 0 is a first-order differential operator; that is, such a sum is equal to a linear combination of $F(a, b, c, z)$ and $F(a+1, b+1, c+1, z)$. In Sec. 12.5 we shall find that matrix elements can equal such a sum and that z and some of the parameters may be complex. It is therefore important in computing to be able to reduce the number of hypergeometric functions and the above idea systematizes this reduction.

Such an argument can be applied to any contiguous solutions of an eigenvalue problem which can be factorized. It is therefore pertinent to ask "when do such recurrence relations themselves represent a direct factorization of the original equation?"

This question can be answered in the following way. We note that the transformation (2.1.2) of a differential equation to the standard form is essentially unique. This means that once λ (the parameter to be held constant on the ladder) has been chosen, the $r(x, m)$ is uniquely determined. For such a definite $r(x, m)$ we have at most one factorization. Therefore we cannot, for example, obtain a factorization of Legendre's equation which will change m by 2 for fixed λ even though there exist first-order differential operators connecting Y_l^m and Y_l^{m+2}.

The situation is the same in the case of the hypergeometric equation: once we had chosen λ (in (4.9.3), λ was $(a-b)^2$) and inserted m, the factorization was determined. But with the hypergeometric equation there is a greater variety of possible choices for λ which might be of interest. For example we could ask if there is a factorization which lowers a and raises b each by 1 at the same time; this would correspond perhaps to taking $\lambda=(a+b)^2$ or perhaps simply $\lambda=c$.

We shall find that there is such a factorization and that

$$\lambda=-(c-1)^2/2-(a+b-c)^2/2. \qquad (4.9.8)$$

However, the problem is type E and so we will leave its discussion to a later section (7.5).

The resulting connection between the fundamental types A and E will be taken up in Chapter 14.

5. Type *B* and *C* Factorizations

From (3.1.1), (3.1.3), (3.1.6), and (3.1.7b, c) respectively, we obtain the next two general factorization types:

Type B (after writing a in place of $-ia$, and adding $-a^2c^2$ to $L(m)$)

$$r(x, m)=-d^2\exp(2ax)+2ad(m+c+\tfrac{1}{2})\exp(ax) \qquad (5.0.1)$$
$$k(x, m)=d\exp(ax)-m-c$$
$$L(m)=-a^2(m+c)^2.$$

Type C (after writing c for d, and adding $b/2$ to $L(m)$)

$$r(x, m)=-(m+c)(m+c+1)/x^2 - b^2x^2/4+b(m-c) \qquad (5.0.2)$$
$$k(x, m)=(m+c)/x+bx/2$$
$$L(m)=-2bm+b/2.$$

We will consider these two types together because any problem which can be treated as type B can also be treated as type C and vice versa; in each case one of the two factorizations will, however, be artificial. Our first example—the confluent hypergeometric equation—is treated in detail by each method and, as we should expect, the two sets of solutions differ only in their normalizations. Subsequent examples will be handled only by the method which preserves the physically proper normalization; it is, fortunately, the more direct method in each case.

Later, in Chapter 8, we shall find that the confluent hypergeometric equation can also be considered as a type F problem.

5.1 Confluent hypergeometric functions

Whittaker and Watson (53) discuss the equation

$$\frac{d^2W}{dz^2}+\left\{-\frac{1}{4}+\frac{s+\frac{1}{2}}{z}+\frac{\frac{1}{4}-m^2}{z^2}\right\}W=0, \quad 0\leq z<\infty \qquad (5.1.1)$$

where we have written $s+\frac{1}{2}$ for their k so that this parameter will not be confused with the $k(x, m)$ function of our factorization. For a factorization which provides s-changing operators we want to treat $-m^2$ as λ. The substitutions

$$z=\exp x, \quad W(z)\sim\exp(x/2)U(x) \qquad (5.1.2)$$

bring (5.1.1) to the desired normal form:

$$\frac{d^2U}{dx^2}+\{-\exp(2x)/4+(s+\tfrac{1}{2})\exp x\}U-m^2U=0, \qquad -\infty<x<\infty. \qquad (5.1.3)$$

We recognize this problem as type B (5.0.1) with $a=1$, $c=0$, $d=\frac{1}{2}$ and with m, λ replaced by s, $-m^2$ respectively. Therefore

$$k(x, s)=(\exp x)/2-s$$
$$L(s)=-s^2.$$

$L(s)$ is a decreasing function of s. Let us consider m (rather than l of Theorem IV) as the smallest value of s; our notation is then consistent with (5.1.3). We now look for quadratically integrable solutions

$$U_m{}^m,\ U_m{}^{m+1},\ U_m{}^{m+2},\ \cdots U_m{}^s,\ \cdots.$$

These solutions are

$$U_m{}^m=\Gamma^{-\frac{1}{2}}(2m)\exp[mx-(\exp x)/2],\quad m>0 \tag{5.1.4a}$$

$$U_m{}^s=[(s-m)(s+m)]^{-\frac{1}{2}}\times\left\{(\exp x)/2-s-\frac{d}{dx}\right\}U_m{}^{s-1} \tag{5.1.4b}$$

$$U_m{}^{s-1}=[(s-m)(s+m)]^{-\frac{1}{2}}\times\left\{(\exp x)/2-s+\frac{d}{dx}\right\}U_m{}^s. \tag{5.1.4c}$$

where the normalization preserved is

$$\int_{-\infty}^{\infty}(U_m{}^s)^2dx=1. \tag{5.1.5}$$

Writing $s=k-\frac{1}{2}$, $z=\exp x$ and using a bar to indicate that our normalization is different than Whittaker and Watson's we obtain

$$U_m{}^s(x)=z^{-\frac{1}{2}}\bar{W}_{k,m}(z).$$

Rewriting (5.1.4) in terms of $\bar{W}$ and z we obtain

$$\bar{W}_{m+\frac{1}{2},m}(z)=\Gamma^{-\frac{1}{2}}(2m)z^{m+\frac{1}{2}}\exp(-z/2) \tag{5.1.6a}$$

$$\bar{W}_{k,m}(z)=[(k-m-\tfrac{1}{2})(k+m-\tfrac{1}{2})]^{-\frac{1}{2}}\times\left\{\frac{z}{2}-k+1-z\frac{d}{dz}\right\}\bar{W}_{k-1,m}(z) \tag{5.1.6b}$$

$$\bar{W}_{k-1,m}(z)=[(k-m-\tfrac{1}{2})(k+m-\tfrac{1}{2})]^{-\frac{1}{2}}\times\left\{\frac{z}{2}-k+z\frac{d}{dz}\right\}\bar{W}_{k,m}(z) \tag{5.1.6c}$$

where the normalization is

$$\int_0^{\infty}(\bar{W}_{k,m}{}^2/z^2)dz=1.$$

Let us now approach our problem as if s were the parameter in (5.1.1) to be held constant (as was λ in the general discussion of Chapter 2) and look for a factorization which provides m-changing operators.

The substitutions

$$z=y^2/4,\quad W(z)\sim(y/2)^{\frac{1}{2}}V(y) \tag{5.1.7}$$

introduce the new normal form

$$\frac{d^2V}{dy^2}-[(2m-\tfrac{1}{2})(2m+\tfrac{1}{2})/y^2+y^2/16]V+(s+\tfrac{1}{2})V=0. \tag{5.1.8}$$

But this equation is almost type C (5.0.2). We can make use of the idea of artificial factorization and write

$$\frac{d^2V}{dy^2}-[(m+\mu-\tfrac{1}{2})(m+\mu+\tfrac{1}{2})/y^2+y^2/16+(m-\mu+\tfrac{1}{2})/2]V+s'V=0 \tag{5.1.9}$$

where $s'=s+\frac{3}{4}+(m-\mu)/2$. This modified equation is exactly type C with $b=-\frac{1}{2}$, $c=\mu-\frac{1}{2}$ and it reduces to (5.1.8) when $\mu=m$. The factorization is given by

$$k(y,m)=(m+\mu-\tfrac{1}{2})/y-y/4$$
$$L(m)=m-\tfrac{1}{4}$$

and the only possible quadratically integrable solutions belonging to a fixed

$$s'=L(l+1)=l+\tfrac{3}{4}$$

are

$$V_l{}^l(\mu),\quad V_l{}^{l-1}(\mu),\quad \cdots V_l{}^m(\mu)\cdots$$

where

$$V_l{}^l(\mu)=2^{-l-\mu-\frac{1}{2}}\Gamma^{-\frac{1}{2}}(l+\mu+1)y^{l+\mu+\frac{1}{2}}\times\exp(-y^2/8) \tag{5.1.10a}$$

$$V_l{}^m(\mu)=[l-m]^{-\frac{1}{2}}\times\left\{(m+\mu+\tfrac{1}{2})/y-y/4+\frac{d}{dy}\right\}V_l{}^{m+1}(\mu). \tag{5.1.10b}$$

Finally, for the required solution of (5.1.8) we merely put $\mu=m$ and $l=s$ in $V_l{}^m(\mu)$; thus s must be an integer $\geq m$.

Using (5.1.7) we obtain the formulas for the corresponding W functions:

$$W^{\mu}{}_{k,k-\frac{1}{2}}(z)=\Gamma^{-\frac{1}{2}}(k+\mu+\tfrac{1}{2})z^{(k+\mu+\frac{1}{2})/2}\exp(-z/2) \tag{5.1.11a}$$

$$W^{\mu}{}_{k,m}(z)=\left[\frac{2k-m-\mu-1}{2}\right]^{-\frac{1}{2}}\left\{\frac{m+\mu}{2z^{\frac{1}{2}}}-\frac{z^{\frac{1}{2}}}{2}+z^{\frac{1}{2}}\frac{d}{dz}\right\}W^{\mu}{}_{k,m+1}(z) \tag{5.1.11b}$$

$$W^{\mu}{}_{k,m+1}(z)=\left[\frac{2k-m-\mu-1}{2}\right]^{-\frac{1}{2}}\left\{\frac{m+\mu+1}{2z^{\frac{1}{2}}}-\frac{z^{\frac{1}{2}}}{2}-z^{\frac{1}{2}}\frac{d}{dz}\right\}W^{\mu}{}_{k,m}(z) \tag{5.1.11c}$$

where the normalization preserved is

$$\int_0^\infty [W^{\mu}{}_{k,m}(z)]^2 dz = 1$$

so that we cannot use an equality sign in

$$W_{k,m}{}^m(z) \sim \bar{W}_{k,m}(z). \tag{5.1.12}$$

We cannot put $\mu = m$ in (5.1.11) since m changes with each step up or down the ladder while μ is held constant and is only put equal to the *final* value of m as in (5.1.12).

Finally, we should note that (5.1.9) is also type C with $b=\frac{1}{2}$, $c=\mu-\frac{1}{2}$ but this choice of b does not lead to integrable solutions.

5.2 Morse potential

Morse (34) has suggested that the radial part of the nuclear wave function (multiplied by r) for a diatomic molecule satisfies

$$\frac{d^2R}{du^2}+\frac{2M}{\hbar^2}\left[E-D(\exp(-2au)-2\exp(-au))-\frac{J(J+1)\hbar^2}{2Mr^2}\right]R=0 \tag{5.2.1}$$

where M is the reduced mass of the two atoms, E the energy, D the "depth" of the potential function and J the rotational quantum number. The constants a, D are to be determined by fitting experimental data to the expression (5.2.3) for the energy levels. The independent variable is $u=r-r_0$ where r is the internuclear distance and r_0 is the value of r when the potential is a minimum. The range for u is $(-r_0, \infty)$ but a sufficiently close approximation is obtained if we take the range to be $(-\infty, \infty)$ since, in this case, R will be extremely small at $r=0$.

As a first approximation we take $J=0$ and then, if we put

$$x=-au+\log[(8MD)^{\frac{1}{2}}/(a\hbar)]$$
$$s+\tfrac{1}{2}=(2MD)^{\frac{1}{2}}/(a\hbar)$$
$$m^2=-2ME/(a^2\hbar^2)$$

(5.2.1) becomes

$$\frac{d^2R}{dx^2}+\{-(\tfrac{1}{4})\exp(2x)+(s+\tfrac{1}{2})\exp x\}R-m^2R=0 \tag{5.2.2}$$

which is Eq. (5.1.3) again. Of course s is not an integer here but it is sufficient that $s-m=\nu=0, 1, 2, \cdots$ which leads to

$$E_\nu=-D+\hbar a(\nu+\tfrac{1}{2})(2D)^{\frac{1}{2}}/M^{\frac{1}{2}}-(\hbar a)^2(\nu+\tfrac{1}{2})^2/(2M) \tag{5.2.3}$$

in agreement with the result given by Morse. We note that there are only a finite number of energy levels—for any given s there are less than $s+1$ levels.

It would be natural to use the m (or ν) changing recurrence relations (5.1.11) to generate the solutions since s is a constant. However the s-changing relation in (5.1.4) preserves the physically correct normalization (once we account for the a in $dx=-adu$). To reach $R_m{}^s$, then, we start with the "solution" $R_m{}^m$ and take ν steps up the s-changing (artificial) ladder to

$$R_m{}^{m+\nu}=R_m{}^s.$$

Moreover we need (5.1.4) for the calculation of intensities in Sec. 10.1.

The potential considered above has been applied to the deuteron problem by Morse, Fisk, and Schiff (35). However, we cannot use the factorization method to solve their problem because r_0 is so small for the deuteron that we can no longer assume the range $(-\infty, \infty)$ for u. D. ter Haar (20) has investigated the limits to the validity of the assumption we have made.

5.3 System of identical oscillators

Schrödinger (42) introduces the equation for a system of s identical (one-dimensional) Planck oscillators. After splitting off the spherical harmonics on the $(s-1)$-dimensional hypersphere he obtains

$$\frac{d^2\psi}{dx^2}+\frac{s-1}{x}\frac{d\psi}{dx}-\left[\frac{n(n+s-2)}{x^2}+x^2\right]\psi+\lambda\psi=0, \qquad n=0, 1, 2, \cdots \tag{5.3.1}$$

for the radial eigenfunction. Here the square of the radius vector is

$$x^2=\sum_1^s x_k{}^2$$

where x_k is the coordinate of the kth oscillator.

By means of the substitution

$$\psi=x^{(1-s)/2}\Phi$$

we change (5.3.1) into its standard form:

$$\frac{d^2\Phi}{dx^2}-[(n+s/2-\tfrac{1}{2})(n+s/2-\tfrac{3}{2})/x^2+x^2]\Phi+\lambda\Phi=0; \tag{5.3.2}$$

this equation is type C with $b=-2$, $c=s/2-\frac{3}{2}$ provided we introduce the artificial $\lambda'=\lambda+2n-s+3$. The factorization leads to the Class I solutions

$$\Phi_l{}^l=2^{\frac{1}{2}}\Gamma^{-\frac{1}{2}}(l+s/2)x^{l+s/2-\frac{1}{2}}\exp(-x^2/2)$$

$$\Phi_l{}^n=(\tfrac{1}{2})[l-n]^{-\frac{1}{2}}\left\{(n+s/2-\tfrac{1}{2})/x-x+\frac{d}{dx}\right\}\Phi_l{}^{n+1}$$

belonging to $\lambda'=4l+3$. That is, $\Phi_l{}^n$ is the normalized eigenfunction belonging to the eigenvalue $\lambda=4l-2n+s$.

Of course an l- (or λ-) changing factorization can be found in the same manner as was the k-changing factorization of Sec. 5.1. The operators provided by such a factorization will raise and lower l by one, and hence λ by 4; the result is essentially that given by Schrödinger.

5.4 Bessel functions

One last example of a type C factorization is important because of a very special property of the $L(m)$ function.

The equation for Bessel function densities is

$$\frac{d^2Z}{dx^2}-\frac{m^2-\frac{1}{4}}{x^2}Z+\lambda Z=0. \tag{5.4.1}$$

The factorization is given by

$$k(x, m)=(m-\tfrac{1}{2})/x$$
$$L(m)=0.$$

Since $L(m)$ is neither increasing nor decreasing as a function of m we have no *key* function. We obtain only the known recurrence formulas:[7]

$$Z_{m+1}=\lambda^{-\frac{1}{2}}\left\{(m+\tfrac{1}{2})/x-\frac{d}{dx}\right\}Z_m$$

$$Z_m=\lambda^{-\frac{1}{2}}\left\{(m+\tfrac{1}{2})/x+\frac{d}{dx}\right\}Z_{m+1}$$

where

$$Z_m=x^{\frac{1}{2}}J_m(\lambda^{\frac{1}{2}}x)$$

in the notation of Whittaker and Watson (53). The recurrence relations also hold for the other solutions of Bessel's equation given by Whittaker and Watson.

6. Type *D* Factorizations

From (3.1.1), (3.1.3), (3.1.6), and (3.1.7d) we obtain the fourth general factorization type. Corresponding to

$$r(x, m)=-(bx+d)^2+b(2m+1) \tag{6.0.1}$$

the factorization is given by

$$\left.\begin{aligned}k(x, m)&=bx+d\\ L(m)&=-2bm\end{aligned}\right\} \tag{6.0.2}$$

where b, d are constants.

The harmonic oscillator problem can be solved by means of this factorization. However, in this case, a straightforward application of the techniques developed in previous chapters and used with all other examples leads to an unnecessarily complicated artificial factorization. The reason is that, for the oscillator, $r(x, m)$ does not depend on m. If m does not appear in the potential function we expect only a *single* ladder of solutions with each function on the ladder belonging to a different eigenvalue of λ. The procedure we have been using, on the other hand, leads to an *infinite number* of ladders, one ladder corresponding to each value of λ and one function on each ladder corresponding to each value of m; but with the oscillator problem these ladders turn out to be identical.

To avoid this duplication we will introduce a slight modification of the factorization procedure in this chapter. The modified version will be simpler and, as a matter of fact, the factorization method had its origin in this treatment of the harmonic oscillator (see, for example, 9, p. 133).

The field of application of the method, as exhibited in this case, is wider than we have so far indicated and embraces many problems which arise during applications of the so-called second quantization procedure. We shall show, with a few examples, how the method can be applied to such problems; but its range of validity is broader than these examples would indicate. We shall also find that the method is easily generalized[8] to handle problems involving sources as well as fields. This generalization is carried out in two stages, in Secs. 6.5 and 6.7. Our examples are formulated and interpreted more fully in Wentzel's *Quantum Theory of Fields* (50).

6.1 Linear oscillator

The Schrödinger equation for an oscillator is

$$\frac{d^2\psi}{d\xi^2}-\xi^2\psi+\lambda\psi=0 \tag{6.1.1}$$

where $\xi=(\hbar/\mu\omega)^{\frac{1}{2}}x$, $\lambda=2E/\hbar\omega$ in the usual notation.

We shall now outline the modified factorization theory which is most suited to this problem. The essential change is that, because 6.1.1 does not depend on m, we now use a factorization which enables us to raise and lower λ.[9]

Equation (6.1.1) can be written in either of the two forms

$$^{+}H\,^{-}H\psi=(\lambda+1)\psi \tag{6.1.2a}$$

$$^{-}H\,^{+}H\psi=(\lambda-1)\psi \tag{6.1.2b}$$

where

$$^{\pm}H=\xi\pm\frac{d}{d\xi}. \tag{6.1.2c}$$

[7] We can, however, obtain explicit expressions for the solutions when m is a half odd integer. For, obviously,

$$Z_{\frac{1}{2}}=\begin{cases}\sin\lambda^{\frac{1}{2}}x\\ \cos\lambda^{\frac{1}{2}}x\end{cases}$$

and the other half odd integral Bessel functions can be gained from these solutions by repeated applications of the recurrence relations.

[8] Johnson and Lippmann (30, 31) have used another generalization (10, p. 136) of Sec. 6.1 to treat the problem of the motion of a charged particle in a uniform magnetic field in both relativistic and nonrelativistic quantum theory.

[9] The idea of raising and lowering λ rather than m persists in Schrödinger's method (41, 42) even in cases where the m does appear.

Operating on (6.1.2a) with ^{-}H and on (6.1.2b) with ^{+}H we deduce the analog of Theorem I:

$$\psi(\lambda+2)\sim{}^{-}H\psi(\lambda)$$
$$\psi(\lambda-2)\sim{}^{+}H\psi(\lambda)$$

so that the $^{\pm}H$ operators raise or lower λ by 2.

Moreover, corresponding to the second part of Theorem IV, we find that we cannot lower the value of λ indefinitely. For the ladder to have a "bottom" we then find that

$$\lambda=2N+1, \quad N=0, 1, 2, \cdots \tag{6.1.3}$$

the key function must satisfy

$$^{+}H\psi_0=0$$

and, properly normalized, it is

$$\psi_0=\pi^{-\frac{1}{4}}\exp(-\xi^2/2). \tag{6.1.4a}$$

The other solutions can then be obtained from the first of

$$\psi_{N+1}=[2N+2]^{-\frac{1}{2}}\,{}^{-}H\psi_N \tag{6.1.4b}$$

$$\psi_{N-1}=[2N]^{-\frac{1}{2}}\,{}^{+}H\psi_N. \tag{6.1.4c}$$

All these eigenfunctions are orthogonal and normalized, that is

$$\int_{-\infty}^{\infty}\psi_N\psi_{N'}d\xi=(\psi_N, \psi_{N'})=\delta_{NN'}.$$

In the next three sections we shall use these results to treat problems arising in the theory of meson fields. With this in mind, we remark that (6.1.2b), and hence (6.1.1), can be written

$$(^{-}H\,{}^{+}H+1)\psi=\lambda\psi. \tag{6.1.5}$$

Thus all our results follow from this one equation.

6.2 Real scalar meson field

The Hamiltonian for a real scalar meson field in vacuum is (50, p. 33)

$$H=(\tfrac{1}{2})\textstyle\sum_k(p_k{}^{*}p_k+\omega_k{}^{2}q_k{}^{*}q_k) \tag{6.2.1}$$

where $\omega_k=c(\mu^2+k^2)^{\frac{1}{2}}>0$ and where k is a vector whose cartesian components are integral multiples of $2\pi/l$, l being the length of the edge of a periodicity cube (50, p. 27). The operators p_k, q_k must satisfy the relations

$$q_{-k}=q_k{}^{*}, \quad p_{-k}=p_k{}^{*} \tag{6.2.2a}$$

$$[q_k, q_{k'}]=[p_k, p_{k'}]=0, \quad [p_k, q_{k'}]=(\hbar/i)\delta_{kk'}. \tag{6.2.2b}$$

Let us now associate with each vector k a one-dimensional space with the coordinate ξ_k where ξ_k ranges from $-\infty$ to $+\infty$, and let us introduce the representation

$$\left.\begin{aligned} q_k&\rightarrow(\hbar/4\omega_k)^{\frac{1}{2}}(^{-}H_k+{}^{+}H_{-k})\\ q_k{}^{*}&\rightarrow(\hbar/4\omega_k)^{\frac{1}{2}}(^{+}H_k+{}^{-}H_{-k})\\ p_k&\rightarrow-(-\hbar\omega_k/4)^{\frac{1}{2}}(^{+}H_k-{}^{-}H_{-k})\\ p_k{}^{*}&\rightarrow(-\hbar\omega_k/4)^{\frac{1}{2}}(^{-}H_k-{}^{+}H_{-k})\end{aligned}\right\} \tag{6.2.3}$$

where

$$^{\pm}H_k=\xi_k\pm\frac{\delta}{\delta\xi_k}.$$

It is easily verified that (6.2.2) is satisfied.

Introducing (6.2.3) into (6.2.1) we obtain

$$H=\textstyle\sum_k(\hbar\omega/2)(^{-}H_k\,{}^{+}H_k+1). \tag{6.2.4}$$

Since the part of the Hamiltonian belonging to each k depends on a separate variable we can split our problem into an infinite number of one-dimensional problems. The Schrödinger equation belonging to each k becomes

$$(\hbar\omega_k/2)(^{-}H_k\,{}^{+}H_k+1)\psi=E_k\psi.$$

A comparison with (6.1.5, 3) gives immediately

$$E_k=\hbar\omega_k(N_k+\tfrac{1}{2})$$

or, subtracting the zero point energy, we obtain

$$E_k'\equiv E_k-\hbar\omega_k/2=\hbar\omega_kN_k$$

and

$$E'\equiv\textstyle\sum_kE_k'=\sum_k\hbar\omega_kN_k. \tag{6.2.5}$$

The eigenfunctions can be obtained from (6.1.4).

Thus the problem of a real scalar, or neutral, meson field is equivalent to that of an oscillator with 3∞ degrees of freedom.

The expression

$$\psi=\psi_{N_k}\psi_{N_{k'}}\cdots \tag{6.2.6}$$

is, symbolically, a solution of the Schrödinger equation

$$H\psi=E\psi, \quad E=\textstyle\sum_kE_k.$$

In (6.2.6) each ψ_{N_k} is normalized to unity exactly as in Sec. 6.1 and it is understood that

$$(\psi, \psi')=\delta_{N_kN'_k}\delta_{N_{k'}N'_{k'}}\cdots$$

where ψ, ψ' are characterized by

$$N_k, \ N_{k'}\cdots$$

and

$$N_k', N'_{k'}\cdots$$

respectively.

6.3 Complex scalar meson field

The Hamiltonian for a complex scalar meson field is (50, p. 51)

$$H=\textstyle\sum_k(p_k{}^{*}p_k+\omega_k{}^{2}q_k{}^{*}q_k). \tag{6.3.1}$$

The difference between this Hamiltonian and that of the previous section is that p_k, q_k no longer satisfy (6.2.2a); they still satisfy (6.2.2b). Physically this means that the charge is no longer zero so that our solutions will represent a field of charged mesons.

With every k we must now associate *two* space coordinates ξ_k, η_k and introduce

$$^{\pm}H_k=\xi_k\pm(\delta/\delta\xi_k)$$
$$^{\pm}L_k=\eta_k\pm(\delta/\delta\eta_k).$$

If we now write

$$\left.\begin{aligned} q_k &\to (\hbar/4\omega_k)^{\frac{1}{2}}(-H_k + {}^+L_k) \\ q_k^* &\to (\hbar/4\omega_k)^{\frac{1}{2}}({}^+H_k + {}^-L_k) \\ p_k &\to -(-\hbar\omega_k/4)^{\frac{1}{2}}({}^+H_k - {}^-L_k) \\ p_k^* &\to (-\hbar\omega_k/4)^{\frac{1}{2}}({}^-H_k - {}^+L_k), \end{aligned}\right\} \tag{6.3.2}$$

Eq. (6.2.3b) is satisfied and our Hamiltonian (6.3.1) becomes

$$H = \sum_k (\hbar\omega_k/2)(-H_k {}^+H_k + {}^-L_k {}^+L_k + 2). \tag{6.3.3}$$

As the partial Hamiltonian belonging to each k depends on separate variables and ξ, η are independent, we can split our problem into one-dimensional problems with Schrödinger equations of the type

$$(\hbar\omega_k/2)(-H_k {}^+H_k + 1)\psi^+ = E^+{}_k \psi^+$$
$$(\hbar\omega_k/2)(-L_k {}^+L_k + 1)\psi^- = E^-{}_k \psi^-.$$

Again, as in 6.1, we have

$$E^+{}_k = \hbar\omega_k(N^+{}_k + \tfrac{1}{2})$$
$$E^-{}_k = \hbar\omega_k(N^-{}_k + \tfrac{1}{2}).$$

The notation $N^+{}_k$, $N^-{}_k$ originates from the fact that we can consider

$$N^+ - N^- = \sum_k (N^+{}_k - N^-{}_k)$$

as proportional to the total charge; $N^+{}_k$ is the number of positively charged mesons with momentum $\hbar k$ and $N^-{}_k$ is the number of negatively charged mesons with momentum $-\hbar k$ (50, p. 53).

6.4 *Many component real theory*

As a last application of the formulas in 6.1 we will sketch the many component theory for which the Hamiltonian is

$$H = \sum_{k,\sigma} (p_k{}^\sigma q_k{}^{*\sigma} + \omega_k{}^2 q_k{}^\sigma q_k{}^{*\sigma})/2 \tag{6.4.1}$$

where

$$q_{-k}{}^\sigma = q_k{}^{*\sigma}, \quad p_{-k}{}^\sigma = p_k{}^{*\sigma}$$

$$[q_k{}^\sigma, q_{k'}{}^{\sigma'}] = [p_k{}^\sigma, p_{k'}{}^{\sigma'}] = 0, \quad [p_k{}^\sigma, q_{k'}{}^{\sigma'}] = \frac{\hbar}{i}\delta_{kk'}\delta_{\sigma\sigma'}.$$

We can treat this problem as we did the one in 6.2. The only difference here is the appearance of the index σ. Thus in analogy to (6.2.3) we introduce

$$q_k{}^\sigma \to (\hbar/4\omega_k)^{\frac{1}{2}}(-H_k{}^\sigma + {}^+H_{-k}{}^\sigma) \text{ etc.}$$

where

$$\pm H_k{}^\sigma = \xi_k{}^\sigma \pm \frac{\delta}{\delta \xi_k{}^\sigma}.$$

Then (6.4.1) becomes

$$\sum_{k,\sigma} (\hbar\omega_k/2)(-H_k{}^\sigma {}^+H_k{}^\sigma + \delta_{\sigma\sigma}). \tag{6.4.2}$$

The one-dimensional Schrödinger equation derived from this problem is

$$(\hbar\omega_k/2)(-H_k{}^\sigma {}^+H_k{}^\sigma + 1)\psi = E_k{}^\sigma \psi. \tag{6.4.3}$$

Therefore

$$E \equiv \sum_{k,\sigma} E_k{}^\sigma = \sum_{k,\sigma} \hbar\omega_k(N_k{}^\sigma + \delta_{\sigma\sigma}/2). \tag{6.4.4}$$

6.5 *Harmonic oscillator; generalization*

So far we have dealt with applications of only the simple factorization (6.1.2). As already stated this factorization is not very different from the general type (6.0.2) quoted at the beginning of this chapter. A glance at the latter suggests that we can generalize our factorization. If in (6.0.2) we now allow the constant d to be a non-zero real number we merely shift the origin and gain nothing new. However, we shall see in the next section that merely allowing d to be a *complex* number β, say, enables us to consider the effect of sources in the (neutral) meson field.

We proceed, then, to consider the consequences of redefining

$$\left.\begin{aligned} {}^+H &= \xi + \beta + (d/d\xi) \\ {}^-H &= \xi + \beta^* - (d/d\xi). \end{aligned}\right\} \tag{6.5.1}$$

Let us also introduce (and this is an essential step) the new operators, complex conjugate to the above:

$$\left.\begin{aligned} {}^+H^* &= \xi + \beta^* + (d/d\xi) \\ {}^-H^* &= \xi + \beta - (d/d\xi). \end{aligned}\right\} \tag{6.5.2}$$

If we attempt to construct a factorization with the first two of these operators we easily find that they enable us to write

$$(d^2\psi/d\xi^2) - \xi^2\psi - (\beta + \beta^*)\xi\psi + (\beta - \beta^*)(d\psi/d\xi) + \lambda\psi = 0 \tag{6.5.3}$$

in either of the two forms

$$\left.\begin{aligned} {}^+H\,{}^-H\psi &= (\lambda + 1 + \beta\beta^*)\psi \\ {}^-H\,{}^+H\psi &= (\lambda - 1 + \beta\beta^*)\psi. \end{aligned}\right\} \tag{6.5.4}$$

The operators (6.5.2) enable us to write

$$(d^2\psi^*/d\xi^2) - \xi^2\psi^* - (\beta + \beta^*)\xi\psi^* - (\beta - \beta^*)(d\psi^*/d\xi) + \lambda\psi^* = 0 \tag{6.5.5}$$

in either of the two forms

$$\left.\begin{aligned} {}^+H^*\,{}^-H^*\psi^* &= (\lambda + 1 + \beta\beta^*)\psi^* \\ {}^-H^*\,{}^+H^*\psi^* &= (\lambda - 1 + \beta\beta^*)\psi^*. \end{aligned}\right\} \tag{6.5.6}$$

Equation (6.5.3) for ψ differs from (6.5.5) for ψ^* only in the sign of the first derivative term; the coefficients of all other terms are real.

The principles of the factorization method can now be applied to (6.5.4) and (6.5.6) but we must treat these factorizations *together*. The reason is that ${}^{+}H$ and ${}^{-}H$ are no longer mutually adjoint; in fact the analog of Theorem II is now

$$\int_{-\infty}^{\infty} \varphi({}^{-}H^{*}f)d\xi = \int_{-\infty}^{\infty} ({}^{+}H\varphi)fd\xi$$

so that Theorem IV for (unnormalized) Class II solutions makes use of the result

$$\begin{aligned}\int_{-\infty}^{\infty} \psi(\lambda-2)\psi^{*}(\lambda-2)d\xi &= \int_{-\infty}^{\infty} {}^{+}H\psi(\lambda)\cdot{}^{+}H^{*}\psi^{*}(\lambda)d\xi \\ &= \int_{-\infty}^{\infty} \psi(\lambda)\,{}^{-}H^{*}\,{}^{+}H^{*}\psi^{*}(\lambda)d\xi \\ &= (\lambda-1+\beta\beta^{*})\int_{-\infty}^{\infty} \psi(\lambda)\psi^{*}(\lambda)d\xi.\end{aligned}$$

It then follows that the eigenvalues are

$$\lambda = 2N+1-\beta\beta^{*}, \quad N=0, 1, 2, \cdots \tag{6.5.7}$$

and the normalized eigenfunctions are given by

$$\left.\begin{aligned}\psi_0 &= \pi^{-\frac{1}{4}}\exp(-(\beta+\beta^{*})^{2}/8-\xi^{2}/2-\beta\xi) \\ \psi_{N+1} &= [2N+2]^{-\frac{1}{2}}\,{}^{-}H\psi_N \\ \psi_{N-1} &= [2N]^{-\frac{1}{2}}\,{}^{+}H\psi_N \\ \psi_0^{*} &= \pi^{-\frac{1}{4}}\exp(-(\beta+\beta^{*})^{2}/8-\xi^{2}/2-\beta^{*}\xi) \\ \psi_{N+1}^{*} &= [2N+2]^{-\frac{1}{2}}\,{}^{-}H^{*}\psi_N^{*} \\ \psi_{N-1}^{*} &= [2N]^{-\frac{1}{2}}\,{}^{+}H^{*}\psi_N^{*}.\end{aligned}\right\} \tag{6.5.8}$$

The normalization now means that

$$\int_{-\infty}^{\infty} \psi_N\psi_{N'}{}^{*}d\xi = (\psi_N, \psi_{N'}) = \delta_{NN'}.$$

For use in the next section we note that if the H operators of 6.1 are now designated by ${}^{\pm}H^{o}$ then

$$-(\beta+\beta^{*})\xi\psi+(\beta-\beta^{*})(d\psi/d\xi) = -\beta\,{}^{-}H^{o}-\beta^{*}\,{}^{+}H^{o}$$

and thus, using (6.1.1, 5), we can rewrite (6.5.3) as

$$({}^{-}H^{o}\,{}^{+}H^{o}+1+\beta\,{}^{-}H^{o}+\beta^{*}\,{}^{+}H^{o})\psi = \lambda\psi. \tag{6.5.9}$$

The factorized form of this equation is (6.5.4). Similarly (6.5.6) is the factorized form of

$$({}^{-}H^{o}\,{}^{+}H^{o}+1+\beta^{*}\,{}^{-}H^{o}+\beta\,{}^{+}H^{o})\psi^{*} = \lambda\psi^{*}. \tag{6.5.10}$$

Thus all our results (6.5.7, 8) follow from either of these last two equations.

6.6 Real scalar meson fields and nucleons

The results of the previous section will now be applied to the problem of a meson field with sources. The simplest theory of the interaction between a neutral meson field and nucleons considers only infinitely heavy nucleons each with the same coupling constant. The Hamiltonian is

$$H = H^{0}+H'. \tag{6.6.1}$$

Here H^{0} is the Hamiltonian (6.2.1) and H' is (50, p. 41)

$$H' = gcV^{-\frac{1}{2}}\sum_{k,n} q_k \exp(ikx_n). \tag{6.6.2}$$

The coupling parameter g has the dimensions of an electric charge; $V=l^{3}$ is the volume of the cube and kx_n is the scalar product of the vector k with the position vector of the nth nucleon.

Let us now introduce into (6.6.2) the operators ${}^{\pm}H^{o}{}_{k}$ for q_k according to (6.2.3). The operator H' becomes

$$\begin{aligned}H' &= \sum_{k,n}(\hbar/4\omega_k)^{\frac{1}{2}}gcV^{-\frac{1}{2}}({}^{-}H^{o}{}_{k}\exp(ikx_n)+{}^{+}H^{o}{}_{-k}\exp(ikx_n)) \\ &= \textstyle\sum_k(\hbar\omega_k/2)(\beta_k\,{}^{-}H^{o}{}_{k}+\beta_k^{*}\,{}^{+}H^{o}{}_{k})\end{aligned}$$

where

$$\begin{aligned}\beta_k &\equiv \textstyle\sum_n \beta_{kn} \\ &\equiv \textstyle\sum_n (2/\hbar\omega_k)(\hbar/4\omega_k)^{\frac{1}{2}}gcV^{-\frac{1}{2}}\exp(ikx_n).\end{aligned}$$

Thus the total Hamiltonian, because of (6.2.4), is

$$\begin{aligned}H = \textstyle\sum_k(\hbar\omega_k/2)({}^{-}H^{o}{}_{k}\,{}^{+}H^{o}{}_{k}+1 \\ +\beta_k\,{}^{-}H^{o}{}_{k}+\beta_k^{*}\,{}^{+}H^{o}{}_{k}).\end{aligned} \tag{6.6.3}$$

Parts of the Hamiltonian belonging to different k's depend on separate variables. Therefore the problem is reduced to that of solving the Schrödinger equation:

$$\begin{aligned}(\hbar\omega_k/2)({}^{-}H^{o}{}_{k}\,{}^{+}H^{o}{}_{k}+1 \\ +\beta_k\,{}^{-}H^{o}{}_{k}+\beta_k^{*}\,{}^{+}H^{o}{}_{k})\psi = E_k\psi.\end{aligned} \tag{6.6.4}$$

Comparing with (6.5.9) we can use (6.5.7) to write down the eigenvalues

$$E_k = \hbar\omega_k(N_k+\tfrac{1}{2})-\hbar\omega_k\beta_k\beta_k^{*}/2.$$

The last term contains the infinite nucleon self energy and the "Yukawa potential function" (50, p. 45).

The expression $\beta_k\beta_k^{*}$ can be split into two parts:

$$\beta_k\beta_k^{*} = \underset{=}{\textstyle\sum_n \beta_{kn}\beta_{kn}^{*}}$$

and

$$\beta_k\beta_k^{*} = \underset{\neq}{\sum_{\substack{n,n' \\ n\neq n'}} \beta_{kn}\beta_{kn'}^{*}}.$$

The first part does not depend on the positions of the nucleons. Thus, introducing

$$E_k' = E_k-\hbar\omega_k/2+\underset{=}{\hbar\omega_k\beta_k\beta_k^{*}/2}$$

we obtain the finite expression

$$E'=\sum_k E_k' = \sum_k \hbar\omega_k(N_k-\beta_k\beta_k^*/2)$$

containing only the energy of the mesons and the mutual energy of the nucleons.

The eigenfunctions are of course obtained from (6.5.8).

6.7 *Further generalization of the oscillator problem*

We consider now one further (and last) generalization of the oscillator problem. This time we allow the d in (6.0.2) to be an *operator* as well as allowing it to be complex. In the next section we shall see how this generalization enables us to consider the effect of sources in a *charged* meson field.

Let us redefine

$$\left.\begin{aligned} {}^{+}H &= \xi+\beta\gamma+\frac{d}{d\xi} \\ {}^{-}H &= \xi+\beta^*\gamma^*-\frac{d}{d\xi} \\ {}^{+}H^* &= \xi+\beta^*\gamma^*+\frac{d}{d\xi} \\ {}^{-}H^* &= \xi+\beta\gamma-\frac{d}{d\xi}. \end{aligned}\right\} \tag{6.7.1}$$

Here β is as before a complex number. But γ, γ^* are operators completely independent of the ${}^{\pm}H^o$ operators. The γ's need not be Hermitian but they must commute.

As in 6.5 we are again able to write down two pairs of factorized equations. They are

$$\left.\begin{aligned} {}^{+}H\,{}^{-}H\psi &= (\lambda+1+\beta\beta^*\gamma\gamma^*)\psi \\ {}^{-}H\,{}^{+}H\psi &= (\lambda-1+\beta\beta^*\gamma\gamma^*)\psi \end{aligned}\right\} \tag{6.7.2a}$$

and

$$\left.\begin{aligned} {}^{+}H^*\,{}^{-}H^*\psi^* &= (\lambda+1+\beta\beta^*\gamma\gamma^*)\psi^* \\ {}^{-}H^*\,{}^{+}H^*\psi^* &= (\lambda-1+\beta\beta^*\gamma\gamma^*)\psi^*. \end{aligned}\right\} \tag{6.7.2b}$$

Because γ, γ^* commute with each other and with ${}^{\pm}H^o$ we can proceed exactly as in 6.5. The results will differ now only in that the eigenvalues and eigenfunctions will be operators (or matrices) since they depend on γ, γ^*.

The eigenvalues are

$$\lambda=(2N+1)I-\beta\beta^*\gamma\gamma^* \tag{6.7.3}$$

where I is the unit operator (or matrix). The eigenfunctions are

$$\left.\begin{aligned} \psi_0 &= A\exp(-\xi^2/2-\beta\gamma\xi) \\ \psi_{N+1} &= [2N+2]^{-\frac{1}{2}}\,{}^{-}H\psi_N \\ \psi_{N-1} &= [2N]^{-\frac{1}{2}}\,{}^{+}H\psi_N \\ \psi_0^* &= A^*\exp(-\xi^2/2-\beta^*\gamma^*\xi) \\ \psi_{N+1}^* &= [2N+2]^{-\frac{1}{2}}\,{}^{-}H^*\psi_N^* \\ \psi_{N-1}^* &= [2N]^{-\frac{1}{2}}\,{}^{+}H^*\psi_N^* \end{aligned}\right\} \tag{6.7.4}$$

where A, A^* are normalization factors.

In spite of the analogy with 6.5 there are also some differences. One is that λ and ψ, as we mentioned before, are operators. Another is that, in this case, ψ^* cannot be regarded simply as the complex conjugate of ψ; yet it plays a role similar to that played by ψ^* in 6.5. Indeed, we can show as before that

$$\int_{-\infty}^{\infty}\psi_{N+1}\psi_{N+1}^*d\xi=(\psi_{N+1},\psi_{N+1})=(\psi_N,\psi_N). \tag{6.7.5}$$

These expressions will be operators since they are functions of γ, γ^*. But if

$$(\psi_0,\psi_0)=I$$

then all the integrals (6.7.5) will equal I, and the eigenfunctions can be said to be normalized.

For use in the next section we note that (6.7.2a) is the factorized form of

$$({}^{-}H^o\,{}^{+}H^o+1+\beta\gamma\,{}^{-}H^o+\beta^*\gamma^*\,{}^{+}H^o)\psi=\lambda\psi \tag{6.7.6}$$

and (6.7.2b) is the factorized form of

$$({}^{-}H^o\,{}^{+}H^o+1+\beta^*\gamma^*\,{}^{-}H^o+\beta\gamma\,{}^{+}H^o)\psi^*=\lambda\psi^* \tag{6.7.7}$$

so the results (6.7.3, 4) follow from these equations.

6.8 *Charged scalar meson fields and nucleons*

The results of the previous section will now be applied to the problem of a charged meson field with sources. Again the simplest interaction theory assumes stationary nucleons but now, because charge must be conserved, it is also necessary to allow for changes of states of the nucleons (50, p. 55).

The eigenfunctions of the proton-neutron states can be represented by

O_n for the neutron state of the nth nucleon
I_n for the proton state of the nth nucleon.

Let us introduce the operators γ_n, γ_n^* such that

$$\begin{aligned} \gamma_n O_n &= I_n & \gamma_n^* O_n &= 0 \\ \gamma_n I_n &= 0 & \gamma_n^* I_n &= O_n. \end{aligned}$$

If the unit of charge is the elementary charge then the charge operator is

$$e_n=\gamma_n\gamma_n^*$$

since

$$e_nO_n=0=0O_n$$
$$e_nI_n=I_n=1I_n.$$

The eigenvalues of e_n are therefore 0 and 1.

The Hamiltonian representing the interaction between the meson field and the nucleons in this case is (50, p. 57):

$$H'=cV^{-\frac{1}{2}}\sum_{k,n}(g\gamma_nq_k\exp(ikx_n)+g^*\gamma_n^*q_k^*\exp(-ikx_n))$$

where g is a complex number. The interaction between the mesons and the Coulomb field of the protons is neglected.

Introducing ${}^{\pm}H^o{}_k$, ${}^{\pm}L^o{}_k$ for q_k according to (6.3.2) and using (6.3.3) for the Hamiltonian without interaction we obtain, for the total Hamiltonian,

$$H=\sum_{k,n}(\hbar\omega_k/2)({}^{-}H^o{}_k{}^{+}H^o{}_k+{}^{-}L^o{}_k{}^{+}L^o{}_k+2$$
$$+\beta_{kn}\gamma_n{}^{-}H^o{}_k+\beta_{kn}^*\gamma_n^*{}^{+}H^o{}_k$$
$$+\beta_{kn}^*\gamma_n^*{}^{-}L^o{}_k+\beta_{kn}\gamma_n{}^{+}L^o{}_k) \quad (6.8.1)$$

where $\beta_{kn}=gcV^{-\frac{1}{2}}(2/\hbar\omega_k)(\hbar/4\omega_k)^{\frac{1}{2}}\exp(ikx_n)$.

Thus we obtain an eigenvalue problem

$$H\psi=E\psi.$$

The ψ^* equation is gained by interchanging in (6.8.1)

$${}^{\pm}H^o \text{ with } {}^{\pm}L^o$$

or

$$\beta_{kn},\ \gamma_n \text{ with } \beta_{kn}^*,\ \gamma_n^*.$$

Our new problem differs essentially from the problem in 6.6 where the meson field was neutral. Here, since γ_n and $\gamma_{n'}{}^*$ do not commute when $n=n'$ we are not able to split our problem into an infinite number of one-dimensional problems.

We can remove this difficulty as follows. In analogy with 6.6 let us write

$$\sum_n\beta_{kn}\beta_{k'n}{}^*\gamma_n\gamma_n{}^*=\beta_k\beta_{k'}{}^*\gamma\gamma^* \quad (6.8.2)$$

$$\sum_{\substack{n,n'\\ n\neq n'}}\beta_{kn}\beta_{k'n'}{}^*\gamma_n\gamma_{n'}{}^*=\beta_k\beta_{k'}{}^*\gamma\gamma^*. \quad (6.8.3)$$

If we now assume the first expression is zero, which means if we ignore the self terms, we *can* separate the different parts of the Hamiltonian. We obtain equations of the type:

$$\left.\begin{aligned}
&(\hbar\omega_k/2)({}^{-}H^o{}_k{}^{+}H^o{}_k+1+\textstyle\sum_n\beta_{kn}\ \gamma_n\ {}^{-}H^o{}_k+\sum_n\beta_{kn}^*\gamma_n^*{}^{+}H^o{}_k)\psi^+ &&=E^+{}_k\psi^+\\
&(\hbar\omega_k/2)({}^{-}L^o{}_k{}^{+}L^o{}_k+1+\textstyle\sum_n\beta_{kn}\ \gamma_n\ {}^{-}L^o{}_k+\sum_n\beta_{kn}^*\gamma_n^*{}^{+}L^o{}_k)\psi^{-*} &&=E^-{}_k\psi^{-*}\\
&(\hbar\omega_k/2)({}^{-}H^o{}_k{}^{+}H^o{}_k+1+\textstyle\sum_n\beta_{kn}^*\gamma_n^*{}^{-}H^o{}_k+\sum_n\beta_{kn}\ \gamma_n\ {}^{+}H^o{}_k)\psi^{+*} &&=E^+{}_k\psi^{+*}\\
&(\hbar\omega_k/2)({}^{-}L^o{}_k{}^{+}L^o{}_k+1+\textstyle\sum_n\beta_{kn}^*\gamma_n^*{}^{-}L^o{}_k+\sum_n\beta_{kn}\ \gamma_n\ {}^{+}L^o{}_k)\psi^- &&=E^-{}_k\psi^-.
\end{aligned}\right\} \quad (6.8.4)$$

We have assumed (6.8.2) is zero to reduce our problem to these equations. But this same assumption also enables us to solve these equations; indeed, the first two equations can be identified with (6.7.6) and the possibility of obtaining the factorization (6.7.2a) of (6.7.6) depended on $\beta\gamma$ commuting with $\beta^*\gamma^*$. The last two equations can be identified with (6.7.7).

Our assumption thus enables us to use the factorizations (6.7.2) where we write

$${}^{+}H=\xi_k+\textstyle\sum_n\beta_{kn}\gamma_n+\dfrac{\delta}{\delta\xi_k}$$

$${}^{+}L=\eta_k+\textstyle\sum_n\beta_{kn}^*\gamma_n^*+\dfrac{\delta}{\delta\eta_k} \quad \text{etc.}$$

and

$$\beta\beta^*\gamma\gamma^*=\beta_k\beta_k{}^*\gamma\gamma^*.$$

The partial eigenvalues are therefore

$$E^+{}_k=\hbar\omega_k(N^+{}_k+\tfrac{1}{2})-\hbar\omega_k\beta_k\beta_k{}^*\gamma\gamma^*/2$$

$$E^-{}_k=\hbar\omega_k(N^-{}_k+\tfrac{1}{2})-\hbar\omega_k\beta_k\beta_k{}^*\gamma\gamma^*/2.$$

Thus the total additional energy introduced by the interaction of the nucleons is

$$\Delta E=-\sum_k\hbar\omega_k\beta_k\beta_k{}^*\gamma\gamma^*. \quad (6.8.5)$$

This additional energy is an operator and can be represented by a diagonal matrix. For example, with two nucleons, the coordinate system in which (6.8.5) is diagonal can be represented by the eigenfunctions

$$O_1O_2+I_1I_2;\quad O_1O_2-I_1I_2;\quad O_1I_2+O_2I_1;\quad O_1I_2-O_2I_1.$$

In a similar way we can treat other cases. Both the separation of the Hamiltonian and then the possibility of factorizing depend on our assumption of commutability, that is on neglecting the self terms. Our procedure also shows that expressions which do not contain self terms as defined here can only be of the second order.

The situation is somewhat simpler in Kemmer's theory (50, p. 64). There we have the Schrödinger equation:

$$\sum_{k,n,\sigma}(\hbar\omega_k/2)({}^{-}H^{o\sigma}{}_k{}^{+}H^{o\sigma}{}_k+\delta_{\sigma\sigma}$$
$$+\beta_{kn}\tau_n{}^{\sigma}{}^{-}H^{o\sigma}{}_k+\beta_{kn}^*\tau_n{}^{\sigma}{}^{+}H^{o\sigma}{}_k)\psi=E\psi \quad (6.8.6)$$

where

$$\tau_n{}^1=\gamma_n+\gamma_n{}^*$$
$$\tau_n{}^2=i(\gamma_n-\gamma_n{}^*)$$
$$\tau_n{}^3=[\gamma_n{}^*,\ \gamma_n].$$

Again, assuming commutability, we can separate (6.8.6) into equations which are even simpler than those considered in 6.7 since they correspond to the special case $\gamma=\gamma^*$. Indeed we obtain immediately

$$E'\equiv\sum_{k,\sigma} E_k{}'^{\sigma}$$
$$\equiv\sum_{k,\sigma}(\hbar\omega_k/2)(2N_k{}^{\sigma}-\sum_{\substack{n,n'\\ n\neq n'}}\beta_{kn}\beta_{kn'}{}^*\tau_n{}^{\sigma}\tau_{n'}{}^{\sigma}). \quad (6.8.7)$$

Our method can be extended in a similar way to other more complicated cases. But its applicability rests on the possibility of separating the Hamiltonian and then being able to factorize each part; each step is possible only if γ commutes with γ^*.

7. Type *E* Factorizations

From (3.1.1), (3.1.7e), (3.1.8), and (3.1.10) we obtain the next general factorization type. Corresponding to

$$r(x,\ m)=-m(m+1)a^2/\sin^2a(x+p)-2aq\cot a(x+p) \quad (7.0.1)$$

the factorization is given by

$$k(x,\ m)=ma\cot a(x+p)+q/m$$
$$L(m)=a^2m^2-q^2/m^2.$$

Perhaps the most striking feature of this type is that it contains the most flexible of all our $L(m)$ functions. As we shall see, the corresponding eigenvalues can be used to represent molecular energy levels; the various forms of $r(x,\ m)$ are therefore important as possible potential functions.

Of the examples considered immediately, we may note that the first two originally appeared as examples of the factorization method.

7.1 Kepler problem in a hypersphere

Schrödinger (42) considered a very interesting problem, that of a hydrogen-like atom in a spherical space. He derived the equation:

$$\frac{d}{dx}\left(\sin^2x\frac{dS}{dx}\right)+2\nu\sin x\cos xS-m(m+1)S+\lambda\sin^2xS=0 \quad (7.1.1)$$

corresponding to a potential $V\sim\cot x$. The range for $x(=r/R)$ is 0, π and

$$\nu=\mu RZe^2/\hbar^2,\quad \lambda=2\mu ER^2/\hbar^2,$$

R being the radius of the hypersphere.

If we put $Y=\sin xS$ we gain the standard form

$$\frac{d^2Y}{dx^2}+\left(2\nu\cot x-\frac{m(m+1)}{\sin^2x}\right)Y+(\lambda+1)Y=0 \quad (7.1.2)$$

which is type E (7.0.1) with $a=1$, $q=-\nu$, $p=0$.

The Class I solutions turn out to be

$$Y_l{}^l=\left(\frac{2}{l+1}\right)^{l+\frac{3}{2}}\left[\frac{\nu(\nu^2+(l+1)^2(l+1)^2)(\nu^2+(l+1)^2l^2)\cdots(\nu^2+(l+1)^2l^2)}{(2l+2)!(1-\exp(-2\nu\pi/(l+1)))}\right]^{\frac{1}{2}}\sin^{l+1}x\exp(-\nu x/(l+1))$$

$$Y_l{}^{m-1}=\left[\lambda+1-m^2+\frac{\nu^2}{m^2}\right]^{-\frac{1}{2}}\left\{m\cot x-\frac{\nu}{m}+\frac{d}{dx}\right\}Y_l{}^m$$

belonging to the eigenvalues

$$\lambda=l(l+2)-\nu^2/(l+1)^2,\quad m\leq l=0,\ 1,\ 2,\ \cdots$$

or $E=l(l+2)\hbar^2/2\mu R^2-Z^2e^4\mu/2\hbar^2(l+1)^2$.

Since $L(m)$ has no finite upper limit, all the eigenvalues are discrete.

As $R\to\infty$ this spectrum approaches that of the Bohr energy levels. As $Z\to 0$ this spectrum approaches the very dense, but discrete, spectrum of a free particle in a spherical space; in 4.3 we referred to the corresponding results as a special case of generalized spherical harmonics.

The substitutions

$$U=\sin^{\frac{1}{2}}xS,\quad z=\log\tan(x/2)$$

enable us to treat our problem as an artificial type A problem which leads to l-changing, or Class II, recurrence relations; the result is essentially that given by Schrödinger (42). However, we will leave such results to a discussion, in Chapter 14, of the connection between types A and E.

Although the above problem was first solved by the factorization method, Stevenson (45) soon showed that, by making explicit use of the continuity as well as the boundedness of the solutions, the problem could be solved by conventional methods.

7.2 Kepler problem in a space of constant negative curvature

It is interesting to compare the above problem with that in an "open," or Milne, universe of constant negative curvature. We shall find that the corresponding

spectrum consists of a *finite* number of (mostly negative) energy levels in addition to a continuous spectrum.

The equation is (28)

$$\frac{d}{dx}\left(\sinh^2 x\frac{dS}{dx}\right)+2\nu\sinh x(\cosh x-\sinh x)S$$
$$-m(m+1)S+\lambda\sinh^2 xS=0 \quad (7.2.1)$$

corresponding to a potential $V\sim(\coth x-1)$ and where ν, λ are as in 7.1. The range for x is now $(0, \infty)$.

To obtain the standard form this time we put $Y=\sinh x S$ so that

$$\frac{d^2Y}{dx^2}+\left[\frac{-m(m+1)}{\sinh^2 x}+2\nu\coth x\right]Y$$
$$+(\lambda-1-2\nu)Y=0 \quad (7.2.2)$$

which is type E with $a=i$, $p=0$, $q=-\nu$ and λ replaced by $\lambda-1-2\nu$. The factorization is therefore given by

$$k(x, m)=m\coth x-\nu/m$$
$$L(m)=-m^2-\nu^2/m^2.$$

For $m<\nu^{\frac{1}{2}}$ $L(m)$ is an increasing function of m and so we obtain the Class I solutions

$$Y_l{}^l=(2)^{l+\frac{1}{2}}\left[\frac{\Gamma(\nu/(l+1)+l+2)}{(2l+2)!\Gamma(\nu/(l+1)-l-1)}\right]^{\frac{1}{2}}$$
$$\times\sinh^{l+1}x\exp(-\nu x/(l+1))$$

$$Y_l{}^{m-1}=[\lambda+m^2+\nu^2/m^2]^{-\frac{1}{2}}\left\{m\coth x-\nu/m+\frac{d}{dx}\right\}Y_l{}^m$$

belonging to the eigenvalues

$$\lambda=2\nu-l(l+2)-\nu^2/(l+1)^2 \quad \text{where} \quad m\leq l=0, 1, 2, \cdots l_0$$

where l_0 is the largest integer such that $l_0+1<\nu^{\frac{1}{2}}$. Thus we obtain the finite number of discrete energy levels

$$E=Ze^2/R-\hbar^2 l(l+2)/2\mu R^2-Z^2e^4\mu/2\hbar^2(l+1)^2,$$
$$l=0, 1, 2, \cdots l_0.$$

For $m>\nu^{\frac{1}{2}}$ $L(m)$ is a decreasing function of m and so we might expect to find Class II solutions associated with the corresponding λ. A closer investigation, however, soon reveals the fact that these "solutions" cannot satisfy the boundary conditions.

We are left, then, with only a finite number of discrete energy levels. This number is $l_0+1\approx\nu^{\frac{1}{2}}=(R/a)^{\frac{1}{2}}$ where a is the radius of the first Bohr orbit of the hydrogen-like atom. Taking $R=10^{28}$ cm we find l_0 is a large number of order 10^{18}. The highest discrete energy level lies between $-3\hbar^2/2\mu R^2$ and $\hbar^2/2\mu R^2$ and thus may be either positive or negative.

It can also be shown, by standard methods, that there exists a continuous spectrum for all $E>\hbar^2/2\mu R^2$.

The corresponding l-changing artificial type A factorization is obtained through $U=\sinh^{\frac{1}{2}}x S$, $z=\log\tanh(x/2)$.

7.3 *Manning-Rosen potential*

Manning and Rosen (33) have suggested that the equation[10]

$$\frac{d^2R}{dr^2}+\left[kE-\frac{\beta(\beta-1)\exp(-2r/\rho)}{\rho^2(1-\exp(-r/\rho))^2}+\frac{A\exp(-r/\rho)}{\rho^2(1-\exp(-r/\rho))}\right]R=0, \quad k=8\pi^2M_1M_2/h^2(M_1+M_2)$$

can be used for the study of diatomic molecules in place of the Morse equation (5.2.1). Their equation can be written

$$\frac{d^2R}{dr^2}+\left[\frac{-\beta(\beta-1)a^2}{\sinh^2 ar}+2a\nu\coth ar\right]R$$
$$+(kE-2a\nu)R=0 \quad (7.3.1)$$

where $\nu=[A+\beta(\beta-1)]/2\rho$, $a=1/2\rho$. In this form we recognize the equation as type E with $p=0$, $q=-\nu$, $m=\beta-1$ and a replaced by ai. Since

$$k(r, m)=ma\coth ar-\nu/m$$
$$L(m)=-a^2m^2-\nu^2/m^2$$

we obtain the results as in the previous section. From $\lambda=L(l+1)$ the eigenvalues become finally

$$E=-\frac{1}{k\rho^2}\left[\frac{A-\beta}{2(\beta+v)}-\frac{v(v+2\beta)}{2(\beta+v)}\right]^2$$

as given by Manning and Rosen and where $v=l+1-\beta=0, 1, 2\cdots v_0$; $v_0<[A+\beta(\beta-1)]^{\frac{1}{2}}-\beta$. The corresponding normalized eigenfunctions can be obtained from

$$R_l{}^l=2^{l+\frac{1}{2}}\left[\frac{a\Gamma(\nu/(al+a)+l+2)}{(2l+2)!\Gamma(\nu/(al+a)-l-1)}\right]^{\frac{1}{2}}$$
$$\times\sinh^{l+1}ar\exp(-\nu r/(al+a))$$

$$R_l{}^m=[\lambda+a^2(m+1)^2+\nu^2/(m+1)^2]^{-\frac{1}{2}}$$
$$\times\left\{(m+1)a\coth ar-\nu/(m+1)+\frac{d}{dr}\right\}R_l{}^{m+1}$$

where we have to put $l=v+\beta-1$, $m=\beta-1$ after all operations have been carried out. Since β is a constant we are interested in only one function for each l—namely, the function with $m=\beta-1$.

[10] The positive energy states belonging to the same potential were investigated earlier by Eckart (14).

7.4 Rosen-Morse potential

In a paper entitled "On the vibrations of polyatomic molecules," Rosen and Morse (38) have found it convenient to introduce new exact solutions of the Schrödinger equation. They consider

$$\frac{d^2\psi}{dx^2}+(1/g^2d^2)[-E-B\tanh(x/d)+C\operatorname{sech}^2(x/d)]\psi=0$$
$$g^2=h^2/8\pi^2Md^2.$$

Now, if in type E we put $p=-\pi/2a$ and then replace a by ai, we obtain the following differential equation:

$$\frac{d^2\psi}{dx^2}+[m(m+1)a^2/\cosh^2ax-2aq\tanh ax]\psi+\lambda\psi=0 \quad (7.4.1)$$

and the corresponding factorization:

$$k(x, m)=ma\tanh ax+q/m$$
$$L(m)=-a^2m^2-q^2/m^2.$$

To solve the Rosen-Morse equation, then, we require solutions of this type E problem for only one value of m: the value such that $m(m+1)=C/g^2$.

There are only Class II solutions belonging to

$$\lambda=-a^2l^2-q^2/l^2, \quad l^2>|q/a|.$$

If $m-l=n$ and since m is fixed, there are only a finite number of eigenvalues given by

$$n=0, 1, 2, \cdots<m-|q/a|-\tfrac{1}{2}.$$

In the notation of Rosen and Morse it turns out that

$$-E=-g^2d^2\lambda=[(4C+g^2)^{\frac{1}{2}}-g(2n+1)]^2/4+B^2/[(4C+g^2)^{\frac{1}{2}}-g(2n+1)]^2.$$

The corresponding eigenfunctions are obtained through

$$\psi_l{}^l=\left[\frac{2^{1-2l}a\Gamma(2l)}{\Gamma(l+q/al)\Gamma(l-q/al)}\right]^{\frac{1}{2}}\cosh^{-l}ax\exp(-qx/l), \quad l^2>|q/a|$$

$$\psi_l{}^m=[\lambda+a^2m^2+q^2/m^2]^{-\frac{1}{2}}\left\{ma\tanh ax+q/m-\frac{d}{dx}\right\}\psi_l{}^{m-1}$$

by putting $m=[-g+(g^2+4C)^{\frac{1}{2}}]/2g$, $l=m-n$, $a=1/d$, $q=B/2g^2d$.

7.5 Jacobi polynomials

The Jacobi polynomials are (47, p. 61)

$$P_n{}^{\alpha,\beta}(z)=\binom{n+\alpha}{n}\times F(-n, n+\alpha+\beta+1, \alpha+1, (1-z)/2) \quad (7.5.1)$$

and they satisfy the differential equation

$$(1-z^2)\frac{d^2P}{dz^2}-\{\alpha-\beta+(\alpha+\beta+2)z\}\frac{dP}{dz}+n(n+\alpha+\beta+1)P=0.$$

To obtain a standard form let us write

$$z=\tanh x$$
$$P\sim(1-\tanh x)^{-\alpha/2}(1+\tanh x)^{-\beta/2}Q\equiv\bar{P}, \text{ say.}$$

Then

$$\frac{d^2Q}{dx^2}+\left[\frac{(n+(\alpha+\beta)/2)(n+(\alpha+\beta)/2+1)}{\cosh^2x}-\frac{\alpha^2-\beta^2}{2}\tanh x\right]Q-\frac{\alpha^2+\beta^2}{2}Q=0 \quad (7.5.2)$$

so that the solutions are obtained from those of the previous section by putting $m=n+(\alpha+\beta)/2$, $a=1$, $q=(\alpha^2-\beta^2)/4$. The fact that $\lambda=-(\alpha^2+\beta^2)/2$ merely means that we are considering only the single ladder with $l=(\alpha+\beta)/2$; this value of l satisfies the restriction $l^2>|q/a|$. The parameter m is not fixed as it was in the previous section so we now have an infinite set of eigenfunctions belonging to each fixed value of l and denoted by $n=0, 1, 2, \cdots$.

The solutions are normalized according to

$$\int_{-1}^{1}(1+z)^{\beta-1}(1-z)^{\alpha-1}[\bar{P}_n{}^{\alpha,\beta}(z)]^2dz=1.$$

If the hypergeometric function in (7.5.1) is written $F(a, b, c, z')$ then λ becomes

$$\lambda=-(c-1)^2/2-(a+b-c)^2/2. \quad (4.9.8)$$

In terms of a, b, c, z', the n-changing operators provide new recurrence formulas for the hypergeometric functions; the n-raising operator would lower a and raise b at the same time (see Sec. 4.9).

8. Type F Factorizations

From (3.1.1), (3.1.7f), (3.1.8), and (3.1.10) we obtain the last general factorization type. Corresponding to

$$r(x, m)=-2q/x-m(m+1)/x^2 \quad (8.0.1)$$

the factorization is given by

$$k(x, m)=m/x+q/m$$
$$L(m)=-q^2/m^2.$$

8.1 Kepler problem

The radial equation in the nonrelativistic hydrogen atom problem is

$$\frac{d^2\psi}{dr^2}+\frac{2}{r}\frac{d\psi}{dr}+\frac{2}{r}\psi-\frac{l(l+1)}{r^2}\psi+\lambda\psi=0 \quad (8.1.1)$$

where $l=0, 1, 2, \cdots$, the unit of length is $\hbar^2/\mu e^2 Z$, and

$$\lambda=(2\hbar^2/\mu Z^2 e^4)E$$

in an obvious notation.

With the substitution

$$R=r\psi \tag{8.1.2}$$

we introduce the radial function densities and (8.1.1) becomes

$$\frac{d^2R}{dr^2}+\left[\frac{2}{r}-\frac{l(l+1)}{r^2}\right]R+\lambda R=0. \tag{8.1.3}$$

Our equation is type F (8.0.1) with $q=-1$ and m replaced by l. The Class I solutions belonging to

$$\lambda=-1/n^2, \quad l+1\leq n=1, 2, 3, \cdots \tag{8.1.4}$$

are

$$R_n^{n-1}=(2/n)^{n+\frac{1}{2}}[(2n)!]^{-\frac{1}{2}}r^n \exp(-r/n) \tag{8.1.5a}$$

$$R_n^{l-1}=+\mathfrak{K}_n^l R_n^l \tag{8.1.5b}$$

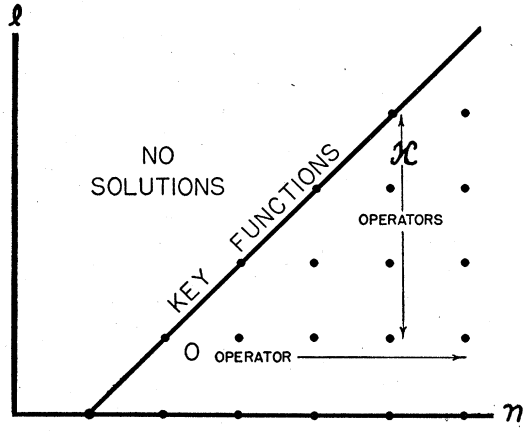


FIG. 3. Each dot represents a solution of the Kepler problem. The solutions are defined by (8.1.5) or, alternatively, by (8.2.1, 2, 3).

where the operator in this case has the form

$$\pm\mathfrak{K}_n^l=nl[(n-l)(n+l)]^{-\frac{1}{2}}\left\{\frac{l}{r}-\frac{1}{l}\pm\frac{d}{dr}\right\},$$

$$=(1/A_n^l)\left\{\frac{l}{r}-\frac{1}{l}\pm\frac{d}{dr}\right\} \tag{8.1.6}$$

for later reference. We will also need the l-raising recurrence formula

$$R_n^l=-\mathfrak{K}_n^l R_n^{l-1}. \tag{8.1.5c}$$

We have written (8.1.4) instead of $\lambda=-1/(n+1)^2$ so that n will be the total quantum number in the usual notation. We are then led immediately to the Bohr formula:

$$E_n=-\mu Z^2 e^4/2\hbar^2 n^2.$$

If $\lambda=1/n^2>0$ the expression $\lambda-L(l+1)$ is always positive so that there is no top for the ladder of solutions and n is therefore not restricted to integral values. The recurrence formulas (8.1.5b, c) are, however, still valid once we replace n by in.

The normalization preserved by (8.1.5) is

$$\int_0^\infty (R_n^l)^2 dr=1$$

i.e.

$$\int_0^\infty (r\psi_n^l)^2 dr=1$$

which is exactly that required by the probability interpretation of the wave functions. Thus the factorization is the natural one for the problem.

The Kepler problem is usually solved by first introducing a new independent variable containing the energy. Putting

$$z=2r/n$$

Eq. (8.1.3), with (8.1.4), becomes

$$\frac{d^2R}{dr^2}+\{-1/4+n/z-l(l+1)/z^2\}R=0$$

which is the same as (5.1.1) for $n=s+\frac{1}{2}$, $l=m-\frac{1}{2}$ and so the solutions are (5.1.6). These type B solutions correspond to Schrödinger's factorization (41). The normalization of these solutions is not the most useful; however, the factorization is important because its recurrence relations can be treated by Truesdell's method whereas (8.1.5) cannot (see Chapter 15).

8.2 New recurrence formula for Kepler functions

In the diagram of Fig. 3 we are able to move up or down by means of the $\mathfrak{K}$ operators of 8.1 or we can move back and forth across the ladders $l=$ constant by means of Schrödinger-type operators, properly interpreted.

We shall now develop a new recurrence formula which enables us to move to the right along the horizontals $l=$ constant: to do this we introduce a new function,

$$R_n^l(s).$$

This function is defined by the same recurrence formula (8.1.5b) as the corresponding function R_n^l. The only difference is that the key functions are now taken to be

$$R_n^{n-1}(s)=(2/n)^{n+\frac{1}{2}}[(2n)!]^{-\frac{1}{2}}r^n \exp(-sr). \tag{8.2.1}$$

Of course the $R_n^l(s)$ are neither orthogonal nor do they satisfy our differential equation, but they have the following important property:

$$[R_n^l(s)]_{s=1/n}=R_n^l. \tag{8.2.2}$$

We can now find an operator which enables us to change $R_n^l(s)$ into $R_{n+1}^l(s)$ from which our solutions

can be got by (8.2.2). In fact

$$\left.\begin{aligned} R_{n+1}{}^{l}(s)&=O_{n+1}{}^{l}R_{n}{}^{l}(s)\\ \text{where}\qquad O_{n+1}{}^{l}&=\frac{n^{l+2}}{(n+1)^{l+2}(2n+1)}\left[\frac{n+l+1}{n-l}\right]^{\frac{1}{2}}\\ &\quad\times\left\{2n+1+(s+1/n)\frac{d}{ds}\right\}.\end{aligned}\right\}\tag{8.2.3}$$

We shall prove this theorem by induction: from (8.1.6) and (8.2.3) it is easily seen that

$${}^{+}\mathcal{K}_{n+1}{}^{l}=\frac{n+1}{n}\left[\frac{(n-l)(n+l)}{(n+1-l)(n+1+l)}\right]^{\frac{1}{2}}{}^{+}\mathcal{K}_{n}{}^{l}$$

and

$$O_{n+1}{}^{l-1}=\frac{n+1}{n}\left[\frac{(n-l)(n+l)}{(n+1-l)(n+1+l)}\right]^{\frac{1}{2}}O_{n+1}{}^{l}.$$

Using (8.1.5b), (8.2.3) and the above equations we find

$$\begin{aligned} R_{n+1}{}^{l-1}(s)&={}^{+}\mathcal{K}_{n+1}{}^{l}R_{n+1}{}^{l}(s)\\ &=\frac{n+1}{n}\left[\frac{(n-l)(n+l)}{(n+1-l)(n+1+l)}\right]^{\frac{1}{2}}{}^{+}\mathcal{K}_{n}{}^{l}O_{n+1}{}^{l}R_{n}{}^{l}(s)\\ &=O_{n+1}{}^{l-1}R_{n}{}^{l-1}(s)\end{aligned}$$

since the $\mathcal{K}$ and O operators commute. Therefore if (8.2.3) is true for the quantum number l it is true for $l-1$. It is a straightforward matter to check that (8.2.3) is true for $l=n-1$; the theorem is then established.

Thus with the help of (8.2.3) we can move to the right along the ladders $l=$ constant. This result is the basis for the calculation of a large class of matrix elements involving Kepler functions which will be taken up in Chapter 12. The essential difference between the O-operator method and the Schrödinger method for changing the energy parameter is that the O-operator commutes with functions of r, differentiation and especially integration with respect to r.

8.3 Generalized Kepler problem

As will be shown in 8.4 the radial part of Dirac's equations for the electron can be solved in terms of generalized Kepler functions. We will therefore present the necessary results in a convenient form.

The generalization needed is, mathematically, a trivial one. In the results of 8.1, 8.2 we have considered n, l to be both integers. However, Theorem IV was based on the milder restriction that the difference between n and l be an integer. All our results will therefore continue to hold if we replace n by $n+\gamma$ and l by $l+\gamma$ where γ is any constant. In particular, the results we need for the solution R of the equation

$$\frac{d^2R}{dr^2}+\frac{2}{r}R-\frac{(l+\gamma)(l+\gamma+1)}{r^2}R-\frac{1}{(n+\gamma)^2}R=0\tag{8.3.1}$$

are

$$R_{n+\gamma}{}^{n+\gamma-1}=(2/(n+\gamma))^{n+\gamma+\frac{1}{2}}\Gamma^{-\frac{1}{2}}(2n+2\gamma+1)r^{n+\gamma}\times\exp(-r/(n+\gamma))\tag{8.3.1a}$$

$$R_{n+\gamma}{}^{l+\gamma-1}={}^{+}\mathcal{K}_{n+1}{}^{l+\gamma}R_{n+\gamma}{}^{l+\gamma}\tag{8.3.1b}$$

$$R_{n+\gamma}{}^{l+\gamma}=-\mathcal{K}_{n+\gamma}{}^{l+\gamma-1}R_{n+\gamma}{}^{l+\gamma-1}\tag{8.3.1c}$$

where

$$\pm\mathcal{K}_{n+\gamma}{}^{l+\gamma}=(n+\gamma)(l+\gamma)[(n-l)(n+l+2\gamma)]^{-\frac{1}{2}}\times\left\{\frac{l+\gamma}{r}-\frac{1}{l+\gamma}\pm\frac{d}{dr}\right\}\tag{8.3.1d}$$

and

$$R_{n+\gamma}{}^{n+\gamma-1}(s)=(2/(n+\gamma))^{n+\gamma+\frac{1}{2}}\Gamma^{-\frac{1}{2}}(2n+2\gamma+1)r^{n+\gamma}\times\exp(-sr)\tag{8.3.2a}$$

$$R_{n+\gamma+1}{}^{l+\gamma}(s)=O_{n+\gamma+1}{}^{l+\gamma}R_{n+\gamma}{}^{l+\gamma}(s)\tag{8.3.2b}$$

where

$$O_{n+\gamma+1}{}^{l+\gamma}=\frac{(n+\gamma)^{l+\gamma+2}}{(n+\gamma+1)^{l+\gamma+2}(2n+2\gamma+1)}\left[\frac{n+l+2\gamma+1}{n-l}\right]^{\frac{1}{2}}\times\left\{2n+2\gamma+1+\left(\frac{1}{n+\gamma}+s\right)\frac{d}{ds}\right\}.\tag{8.3.2c}$$

The above generalization is not entirely trivial for it is now possible that $n=0$. Thus the solution $R_{\gamma}{}^{\gamma-1}$ exists which has no counterpart in the ordinary Kepler problem. Furthermore the other solutions for $l=-1$ can be reached by the operators since the operators (with $l=0$) are no longer singular.

8.4 Dirac's radial functions

The radial functions for the Kepler problem treated by Dirac's theory are the solutions of (2, p. 312):

$$\frac{d\chi_1}{dr}-k\chi_1/r=\{(1-E/E_0)\mu c/\hbar-\alpha Z/r\}\chi_2$$

$$\frac{d\chi_2}{dr}+k\chi_2/r=\{(1+E/E_0)\mu c/\hbar+\alpha Z/r\}\chi_1$$

where k is the auxiliary quantum number and must be an integer, positive or negative, but not zero. $E_0=\mu c$ is the rest energy.

If we introduce

$$\gamma_1=(k-\alpha Z)^{\frac{1}{2}},\quad \gamma_2=(k+\alpha Z)^{\frac{1}{2}},$$
$$\gamma=\gamma_1\gamma_2,\quad \epsilon=E/E_0,\quad b=\mu c/\hbar,\quad a=b\epsilon\alpha Z$$

and

$$\psi_1=(\gamma_1+\gamma_2)\chi_1+(\gamma_1-\gamma_2)\chi_2$$
$$\psi_2=(\gamma_1-\gamma_2)\chi_1+(\gamma_1+\gamma_2)\chi_2$$

and write $ar=x$ (so that the independent variable contains the energy parameter), we obtain

$$\left.\begin{aligned}\left\{\frac{\gamma}{x}-\frac{1}{\gamma}-\frac{d}{dx}\right\}\psi_1&=-\frac{b}{a}\left(\frac{\epsilon k}{\gamma}-1\right)\psi_2\\ \left\{\frac{\gamma}{x}-\frac{1}{\gamma}+\frac{d}{dx}\right\}\psi_2&=-\frac{b}{a}\left(\frac{\epsilon k}{\gamma}+1\right)\psi_1.\end{aligned}\right\}\tag{8.4.1}$$

Now put

$$R_1=(\epsilon k/\gamma+1)^{\frac{1}{2}}\psi_1,\quad R_2=(\epsilon k/\gamma-1)^{\frac{1}{2}}\psi_2\tag{8.4.2}$$

and Eqs. (8.4.1) become exactly (8.3.1b) and (8.3.1c) for $l=0$ provided we identify

$$R_1=R_{n+\gamma}{}^{\gamma-1},\quad R_2=R_{n+\gamma}{}^{\gamma}$$

and

$$(b/a)(\epsilon^2k^2/\gamma^2-1)^{\frac{1}{2}}=[n(n+2\gamma)]^{\frac{1}{2}}/(n+\gamma)\gamma.$$

This last condition leads to the known formula

$$\epsilon=(1+\alpha^2Z^2/(n+\gamma)^2)^{-\frac{1}{2}},\quad n=0,1,2,\cdots.\tag{8.4.3}$$

The possibility $n=0$ must be given special consideration since, in this case, $\epsilon=\gamma/|k|$ (since $\epsilon>0$) and the substitutions (8.4.2) cannot be used. Going back to (8.4.1) it is a simple matter to check that, in this case, the only solutions satisfying the boundary condition are

$$\begin{aligned}k>0\quad&\psi_1=\psi_2=0\\ k<0\quad&\psi_1\neq0,\quad\psi_2=0.\end{aligned}$$

These results are automatically contained in the final formulas for the solutions which are

$$\chi_1=C\{(\gamma_2+\gamma_1)(\epsilon k-\gamma)^{\frac{1}{2}}R_{n+\gamma}{}^{\gamma-1}(x)+(\gamma_2-\gamma_1)(\epsilon k+\gamma)^{\frac{1}{2}}R_{n+\gamma}{}^{\gamma}(x)\}\tag{8.4.4a}$$

$$\chi_2=C\{(\gamma_2-\gamma_1)(\epsilon k-\gamma)^{\frac{1}{2}}R_{n+\gamma}{}^{\gamma-1}(x)+(\gamma_2+\gamma_1)(\epsilon k+\gamma)^{\frac{1}{2}}R_{n+\gamma}{}^{\gamma}(x)\}\tag{8.4.4b}$$

where it remains only to determine the normalization constant C. The condition to be satisfied is

$$\int_0^\infty(\chi_1{}^2+\chi_2{}^2)dr=a^{-1}\int_0^\infty(\chi_1{}^2+\chi_2{}^2)dx=1.$$

Since the R functions are normalized this condition becomes

$$(8C^2/a)\{\epsilon k^2+(\epsilon^2k^2-\gamma^2)^{\frac{1}{2}}\alpha ZI_{n+\gamma}{}^{\gamma-1,\gamma}\}=1$$

where

$$I_{n+\gamma}{}^{\gamma-1,\gamma}=\int_0^\infty R_{n+\gamma}{}^{\gamma-1}R_{n+\gamma}{}^{\gamma}dx.$$

Lin (32) has shown that

$$I_{n+\gamma}{}^{\gamma-1,\gamma}=-(\epsilon^2k^2-\gamma^2)^{\frac{1}{2}}/\alpha Z\epsilon\tag{8.4.5}$$

so that, finally, the normalization factor is

$$C=(\epsilon a/2)^{\frac{1}{2}}/2\gamma.\tag{8.4.6}$$

Lin's ingenious method is as follows: first write

$$\pm H^{l+\gamma}=\left\{\frac{l+\gamma}{x}-\frac{1}{l+\gamma}\pm\frac{d}{dx}\right\}$$

$$A_{n+\gamma}{}^{l+\gamma}=[(n-l)(n+l+2\gamma)]^{\frac{1}{2}}/(n+\gamma)(l+\gamma)$$

and

$$I_{n+\gamma}{}^{l+\gamma-1,l+\gamma}=\int_0^\infty R_{n+\gamma}{}^{l+\gamma-1}R_{n+\gamma}{}^{l+\gamma}dx.$$

Then it is easily checked that

$$-H^{l+\gamma}=\xi_l-H^{l+\gamma-1}+\eta_l+H^{l+\gamma-1}+\zeta_l$$

where

$$\xi_l+\eta_l=(l+\gamma)/(l+\gamma-1),\quad-\xi_l+\eta_l=1$$
$$\zeta_l=(l+\gamma)\{1/(l+\gamma-1)^2-1/(l+\gamma)^2\}$$

so that, making use of Theorem II, we obtain

$$A_{n+\gamma}{}^{l+\gamma}I_{n+\gamma}{}^{l+\gamma-1,l+\gamma}=(\xi_l+\eta_l)A_{n+\gamma}{}^{l+\gamma-1}I_{n+\gamma}{}^{l+\gamma-2,l+\gamma-1}+\zeta_l$$

or

$$A_{n+\gamma}{}^{l+\gamma}I_{n+\gamma}{}^{l+\gamma-1,l+\gamma}/(l+\gamma)+1/(l+\gamma)^2=A_{n+\gamma}{}^{l+\gamma-1}I_{n+\gamma}{}^{l+\gamma-2,l+\gamma-1}/(l+\gamma-1)+1/(l+\gamma-1)^2.$$

Either side must therefore be independent of l and hence equal to $1/(n+\gamma)^2$ since $R_{n+\gamma}{}^{n+\gamma}\equiv0$. Therefore

$$I_{n+\gamma}{}^{\gamma-1,\gamma}=\gamma[1/(n+\gamma)^2-1/\gamma^2]/A_{n+\gamma}{}^{\gamma}=-[1-\gamma^2/(n+\gamma)^2]^{\frac{1}{2}}.$$

Using (8.4.3) for $n+\gamma$ we obtain (8.4.5) as required.

The expressions (8.4.4) can also be interpreted as the solutions for $E>\mu c^2$ provided we replace $n+\gamma$ by $in+i\gamma$ where the value of n will now be unrestricted. We will show in 12.5 that the normalization constant C becomes, in this case,

$$C=(a/2\epsilon)^{\frac{1}{2}}/2\gamma\tag{8.4.7}$$

if the modulus squared of the corresponding eigendifferential is proportional to the number of electrons per unit velocity range. Since there is no key function corresponding to (8.3.1a) for $R_{in+i\gamma}{}^{l+\gamma}$ we have yet to explain how these functions should be normalized. This is done in Sec. 12.5.

8.5 Oscillating rotator

The differential equation for the oscillating rotator is (44)

$$\frac{d^2\Phi}{dr^2}+\frac{2a}{r}\Phi-\frac{l(l+1)+a}{r^2}\Phi+\lambda\Phi=0 \qquad (8.5.1)$$

where a is a given positive parameter.

If we put $ar=x$ and $\gamma=-(l+\frac{1}{2})+((l+\frac{1}{2})^2+a)^{\frac{1}{2}}$ then (8.5.1) becomes (8.3.1) and so the solutions (normalized on the range for r) become

$$\Phi_\lambda{}^l=a^{\frac{1}{2}}R_{n+\gamma}{}^{l+\gamma}(ar)$$

corresponding to the eigenvalue $\lambda=-a^2/(n+\gamma)^2$ i.e. to

$$(-\lambda)^{\frac{1}{2}}=a/[n-l-\tfrac{1}{2}+((l+\tfrac{1}{2})^2+a)^{\frac{1}{2}}],$$
$$l=-1, 0, 1, 2, \cdots\leq n-1.$$

9. Type *A* Matrix Elements

In the next four chapters we are going to consider the problem of calculating certain integrals whose values depend on the eigenfunctions of the preceding chapters. These integrals are the transition probabilities of quantum mechanics.

Our aim is to show how the key function and recurrence relations provided by the factorization method can be used to find quickly the corresponding matrix elements.

9.1 Spherical harmonics

To evaluate spherical harmonic matrix elements it is only necessary to have $\cos\theta Y_l{}^m$ and $\sin\theta Y_l{}^m$ expressed as linear combinations of contiguous solutions. For, with these expressions and the orthogonal and normalization properties of the solutions, we are able to calculate integrals of the form

$$\int_0^\pi \cos^p\theta\,\sin^q\theta Y_l{}^m Y_{l'}{}^{m'}d\theta \qquad (9.1.1)$$

where p, q are integers and we must have $m-m'=-q$, $-q+2, \cdots q$.

Now, the Class I solutions (4.1.4) of the associated spherical harmonics equation satisfy the physically proper normalization condition (4.2.5). To find the expressions required for the calculation of (9.1.1) our first step is to adjust the constants in (4.2.4) so that these Class II recurrence relations preserve the same normalization.

Let us introduce $a_l{}^m$ so that

$$\sin^{-\frac{1}{2}}\theta Y_l{}^m\equiv P_l{}^m\equiv a_l{}^m\bar{P}_l{}^m.$$

That is, $a_l{}^m$ is the correction to the normalization of $\bar{P}_l{}^m$.

We can now rewrite (4.2.4) in terms of $Y_l{}^m$

$$Y_{l+1}{}^m=(a_{l+1}{}^m/a_l{}^m)[(l+1-m)(l+1+m)]^{-\frac{1}{2}}\times\left\{-(l+\tfrac{1}{2})\cos\theta-\sin\theta\frac{d}{d\theta}\right\}Y_l{}^m \qquad (9.1.2a)$$

$$Y_{l-1}{}^m=(a_{l-1}{}^m/a_l{}^m)[(l-m)(l+m)]^{-\frac{1}{2}}\times\left\{-(l+\tfrac{1}{2})\cos\theta+\sin\theta\frac{d}{d\theta}\right\}Y_l{}^m \qquad (9.1.2b)$$

and we have only to find the ratio $a_{l+1}{}^m/a_l{}^m$.

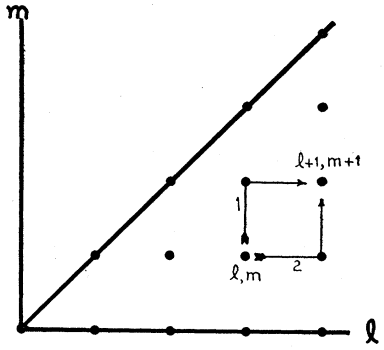


FIG. 4. The solution $Y_{l+1}{}^{m+1}$ can be reached from $Y_l{}^m$ by moving along either path with the appropriate operators.

We can easily show that this ratio is independent of the suffix m. We will do this by comparing the results of moving with our operators along the two paths shown in Fig. 4. In fact we can write either (from path 1):

$$Y_{l+1}{}^{m+1}=(a_{l+1}{}^{m+1}/a_l{}^{m+1})[(l-m)(l+2+m)]^{-\frac{1}{2}}\times\left\{-(l+\tfrac{1}{2})\cos\theta-\sin\theta\frac{d}{d\theta}\right\}Y_l{}^{m+1}$$
$$=(a_{l+1}{}^{m+1}/a_l{}^{m+1})[\cdots]^{-\frac{1}{2}}\{\cdots\}\times[(l-m)(l+m+1)]^{-\frac{1}{2}}\left\{(m+\tfrac{1}{2})\cot\theta-\frac{d}{d\theta}\right\}Y_l{}^m$$

or (from path 2):

$$Y_{l+1}{}^{m+1}=[(l-m+1)(l+m+2)]^{-\frac{1}{2}}\times\left\{(m+\tfrac{1}{2})\cot\theta-\frac{d}{d\theta}\right\}Y_{l+1}{}^m$$
$$=[\cdots]^{-\frac{1}{2}}\{\cdots\}(a_{l+1}{}^m/a_l{}^m)\times[(l+1-m)(l+1+m)]^{-\frac{1}{2}}\times\left\{-(l+\tfrac{1}{2})\cos\theta-\sin\theta\frac{d}{d\theta}\right\}Y_l{}^m.$$

After performing the indicated operations we find that the two right-hand sides above are equal provided

$$a_{l+1}{}^{m+1}/a_l{}^{m+1}=a_{l+1}{}^m/a_l{}^m\equiv a_{l+1}/a_l, \qquad (9.1.3a)$$

say, which we set out to show.

By equating the right-hand sides in the two expressions

$$Y_{l+1}{}^{l}=[2l+2]^{-\frac{1}{2}}\left\{(l+\tfrac{1}{2})\cot\theta+\frac{d}{d\theta}\right\}Y_{l+1}{}^{l+1}$$

$$Y_{l+1}{}^{l}=(a_{l+1}/a_l)[2l+1]^{-\frac{1}{2}}\left\{-(l+\tfrac{1}{2})\cos\theta-\sin\theta\frac{d}{d\theta}\right\}Y_l{}^{l}$$

and using the known expression (4.1.4a) for $Y_l{}^{l}$, $Y_{l+1}{}^{l+1}$ we can easily find the value

$$a_{l+1}/a_l=-(2l+3)^{\frac{1}{2}}/(2l+1)^{\frac{1}{2}}. \tag{9.1.3b}$$

It is now a straightforward matter to find the formulas to be used in calculating matrix elements.

With (9.1.3) in (9.1.2) we obtain

$$\left\{(l+\tfrac{1}{2})\cos\theta+\sin\theta\frac{d}{d\theta}\right\}Y_l{}^{m}=\left[\frac{(l+1-m)(l+1+m)(2l+1)}{2l+3}\right]^{\frac{1}{2}}Y_{l+1}{}^{m} \tag{9.1.4a}$$

$$\left\{(l+\tfrac{1}{2})\cos\theta-\sin\theta\frac{d}{d\theta}\right\}Y_l{}^{m}=\left[\frac{(l-m)(l+m)(2l+1)}{2l-1}\right]^{\frac{1}{2}}Y_{l-1}{}^{m}. \tag{9.1.4b}$$

Adding these two equations and dividing by $2l+1$ we obtain

$$\cos\theta Y_l{}^{m}=\left[\frac{(l+1-m)(l+1+m)}{(2l+1)(2l+3)}\right]^{\frac{1}{2}}Y_{l+1}{}^{m}+\left[\frac{(l-m)(l+m)}{(2l+1)(2l-1)}\right]^{\frac{1}{2}}Y_{l-1}{}^{m} \tag{9.1.5a}$$

which is the first of the expressions required.

To expand $\sin\theta Y_l{}^{m}$ we write

$$\begin{aligned}[(l+m+1)(l-m)]^{\frac{1}{2}}\sin\theta Y_l{}^{m}&=\sin\theta\left\{(m+\tfrac{1}{2})\cot\theta+\frac{d}{d\theta}\right\}Y_l{}^{m+1}\\&=\left\{-(l+\tfrac{1}{2})\cos\theta+\sin\theta\frac{d}{d\theta}\right\}Y_l{}^{m+1}\\&\quad+(m+l+1)\cos\theta Y_l{}^{m+1}\\&=-\left[\frac{(l-m-1)(l+m+1)(2l+1)}{2l-1}\right]^{\frac{1}{2}}Y_{l-1}{}^{m+1}\\&\quad+(m+l+1)\cos\theta Y_l{}^{m+1}.\end{aligned}$$

Dividing by the radical on the left side and using (9.1.5a) we obtain

$$\sin\theta Y_l{}^{m}=\left[\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}\right]^{\frac{1}{2}}Y_{l+1}{}^{m+1}-\left[\frac{(l-m-1)(l-m)}{(2l+1)(2l-1)}\right]^{\frac{1}{2}}Y_{l-1}{}^{m+1}. \tag{9.1.5b}$$

Similarly, by starting with $Y_l{}^{m}$ in terms of $Y_l{}^{m-1}$ we can obtain

$$\sin\theta Y_l{}^{m}=-\left[\frac{(l-m+1)(l-m+2)}{(2l+1)(2l+3)}\right]^{\frac{1}{2}}Y_{l+1}{}^{m-1}+\left[\frac{(l+m-1)(l+m)}{(2l+1)(2l-1)}\right]^{\frac{1}{2}}Y_{l-1}{}^{m-1}. \tag{9.1.5c}$$

The formulas (9.1.5) along with

$$\int_0^{\pi}Y_l{}^{m}Y_{l'}{}^{m}d\theta=\delta_{ll'}$$

are sufficient for the calculation of spherical harmonic matrix elements of the type (9.1.1).

9.2 Generalized spherical harmonics

We can easily adapt the arguments of the preceding section to the solutions of the generalized spherical harmonics equation given in Sec. 4.3.

The corresponding results are as follows:

$$\begin{aligned}a_{l+1,\gamma}{}^{m}/a_{l,\gamma}{}^{m}&=-(l+\gamma+1)^{\frac{1}{2}}/(l+\gamma)^{\frac{1}{2}}\\\cos\theta Y_{l,\gamma}{}^{m}&=\left[\frac{(l-m+1)(l+m+2\gamma)}{4(l+\gamma)(l+\gamma+1)}\right]^{\frac{1}{2}}Y_{l+1,\gamma}{}^{m}+\left[\frac{(l-m)(l+m+2\gamma-1)}{4(l+\gamma)(l+\gamma-1)}\right]^{\frac{1}{2}}Y_{l-1,\gamma}{}^{m}\\\sin\theta Y_{l,\gamma}{}^{m}&=\left[\frac{(l+m+2\gamma)(l+m+2\gamma+1)}{4(l+\gamma)(l+\gamma+1)}\right]^{\frac{1}{2}}Y_{l+1,\gamma}{}^{m+1}-\left[\frac{(l-m-1)(l-m)}{4(l+\gamma)(l+\gamma-1)}\right]^{\frac{1}{2}}Y_{l-1,\gamma}{}^{m+1}\\&=-\left[\frac{(l-m+1)(l-m+2)}{4(l+\gamma)(l+\gamma+1)}\right]^{\frac{1}{2}}Y_{l+1,\gamma}{}^{m-1}+\left[\frac{(l+m+2\gamma-2)(l+m+2\gamma-1)}{4(l+\gamma)(l+\gamma-1)}\right]^{\frac{1}{2}}Y_{l-1,\gamma}{}^{m-1}.\end{aligned}$$

9.3 When the integrand contains three spherical harmonics

We now show how the factorization method can be used to find explicitly the value of

$$\int_0^{\pi}P_{l_1}{}^{m_1}Y_{l_2}{}^{m_2}Y_{l_3}{}^{m_3}d\theta,\quad m_1=m_2+m_3. \tag{9.3.1}$$

This integral (with differently normalized functions) was calculated by Gaunt (17) and similar problems were considered earlier by Adams (1). In applications such integrals have occurred, for example, in a paper by Elsasser (15) on the origin of the earth's magnetic field.

Because of (4.1.2, 4) and Theorem II

$$\int_0^\pi P_{l_1}^{m_1} Y_{l_2}^{m_2} Y_{l_3}^{m_3} d\theta$$

$$= [(l_1-m_1)(l_1+m_1+1)]^{-\frac{1}{2}}$$

$$\times \int_0^\pi \left\{(m_1+1)\cot\theta + \frac{d}{d\theta}\right\} P_{l_1}^{m_1+1} \cdot Y_{l_2}^{m_2} Y_{l_3}^{m_3} d\theta$$

$$= [(l_1-m_1)(l_1+m_1+1)]^{-\frac{1}{2}} \int_0^\pi P_{l_1}^{m_1+1}$$

$$\times \left\{(m_2+\tfrac{1}{2})\cot\theta + (m_3+\tfrac{1}{2})\cot\theta - \frac{d}{d\theta}\right\} Y_{l_2}^{m_2} Y_{l_3}^{m_3} d\theta$$

$$= [(l_1-m_1)(l_1+m_1+1)]^{-\frac{1}{2}} \Big\{ [(l_2-m_2)(l_2+m_2+1)]^{\frac{1}{2}}$$

$$\times \int_0^\pi P_{l_1}^{m_1+1} Y_{l_2}^{m_2+1} Y_{l_3}^{m_3} d\theta$$

$$+ [(l_3-m_3)(l_3+m_3+1)]^{\frac{1}{2}}$$

$$\times \int_0^\pi P_{l_1}^{m_1+1} Y_{l_2}^{m_2} Y_{l_3}^{m_3+1} d\theta \Big\}. \quad (9.3.2)$$

Using this formula altogether l_1-m_1 times, it is a simple matter to write down the general term in the resulting series of integrals. Rearranging only slightly leads to

$$\int_0^\pi P_{l_1}^{m_1} Y_{l_2}^{m_2} Y_{l_3}^{m_3} d\theta$$

$$= \left[\frac{(l_1+m_1)!(l_2-m_2)!(l_3-m_3)!}{(l_1-m_1)!(2l_1)!(l_2+m_2)!(l_3+m_3)!}\right]^{\frac{1}{2}}$$

$$\times \sum_{i=0}^{l_1-m_1} \binom{l_1-m_1}{i}$$

$$\times \left[\frac{(l_2+l_1+m_2-m_1-i)!(l_3+m_3+i)!}{(l_2-l_1-m_2+m_1+i)!(l_3-m_3-i)!}\right]^{\frac{1}{2}}$$

$$\times \int_0^\pi P_{l_1}^{l_1} Y_{l_2}^{m_2+l_1-m_1-i} Y_{l_3}^{m_3+i} d\theta. \quad (9.3.3)$$

The superscripts of at least one of the Y's in each product will be greater than the corresponding subscript and hence the integrals will all vanish unless

$$l_1 \leq l_2 + l_3.$$

From (9.1.5b, c) and since

$$P_{l_1}^{l_1} = \left[\frac{1.3.5\cdots(2l_1+1)}{2.2.4\cdots 2l_1}\right]^{\frac{1}{2}} \sin^{l_1}\theta$$

it is seen that

$$P_{l_1}^{l_1} Y_{l_2}^{m_2+l_1-m_1-i} = (\ ) Y_{l_2-l_1}^{m_3+i} + (\ ) Y_{l_2-l_1+2}^{m_3+i} + \cdots + (\ ) Y_{l_2+l_1}^{m_3+i}$$

where the brackets contain only constants. Now, using the orthogonality property of the Y functions, we see that the integrals in (9.3.3) will all vanish unless

$$l_1+l_2+l_3 = \text{even number}$$
$$l_2-l_1 \leq l_3 \leq l_2+l_1.$$

The selection rules can be summarized by saying the l's must be equal to the sides of a triangle with even perimeter.

The selection rules must be satisfied if (9.3.1) is to be not zero; but the integral may be zero even if the selection rules *are* satisfied due to the possibility of different terms in (9.3.3) cancelling one another. One such exceptional case found by Bird (3) is

$$\int_0^\pi P_3^2 Y_2^0 Y_3^2 d\theta = 0.$$

It remains to evaluate integrals of the form

$$\int_0^\pi \sin^{l_1}\theta Y_{l_2}^{\alpha} Y_{l_3}^{\beta} d\theta, \quad l_1 = \alpha+\beta.$$

For this purpose we need two reduction formulas. The first is obtained from

$$\sin^{l_1}\theta Y_{l_2}^{\alpha} = [(l_2+\alpha+1)(l_2-\alpha)]^{-\frac{1}{2}}$$
$$\times \{(\alpha+\tfrac{1}{2}-l_1)\cot\theta + (d/d\theta)\} \sin^{l_1}\theta Y_{l_2}^{\alpha+1}$$

which follows from (4.1.4b). Then, in a manner analogous to that used in finding (9.3.2), we obtain

$$\int_0^\pi \sin^{l_1}\theta Y_{l_2}^{\alpha} Y_{l_3}^{\beta} d\theta = -\left[\frac{(l_3+\beta)(l_3-\beta+1)}{(l_2+\alpha+1)(l_2-\alpha)}\right]^{\frac{1}{2}}$$
$$\times \int_0^\pi \sin^{l_1}\theta Y_{l_2}^{\alpha+1} Y_{l_3}^{\beta-1} d\theta. \quad (9.3.4)$$

Using this formula $l_2-\alpha$ times we reduce the problem to that of finding

$$\int_0^\pi \sin^{l_1+l_2+\frac{1}{2}}\theta Y_{l_3}^{l_1-l_2} d\theta. \quad (9.3.5)$$

A reduction formula for this integral can be obtained by first multiplying the differential equation (4.1.3) by $\sin^n\theta$ and integrating twice by parts. Then

$$\int_0^\pi \sin^{n-2}\theta Y_l^m d\theta = \frac{(n+l+\frac{1}{2})(n-l-\frac{1}{2})}{(n+m-\frac{1}{2})(n-m-\frac{1}{2})} \times \int_0^\pi \sin^n\theta Y_l^m d\theta, \quad n>\tfrac{1}{2}. \quad (9.3.6)$$

Further

$$\begin{aligned}\int_0^\pi &\sin^n\theta Y_l^m d\theta \\ &= [(l+m+1)(l-m)]^{-\frac{1}{2}} \times \int_0^\pi \sin^n\theta \left\{(m+\tfrac{1}{2})\cot\theta + \frac{d}{d\theta}\right\} Y_l^{m+1} d\theta \\ &= [(l+m+1)(l-m)]^{-\frac{1}{2}} \times \int_0^\pi (m-n+\tfrac{1}{2})\cos\theta \sin^{n-1}\theta Y_l^{m+1} d\theta \\ &= [(l+m+1)(l-m)(l+m+2)(l-m-1)]^{-\frac{1}{2}} \times (m-n+\tfrac{1}{2}) \int_0^\pi [(m-n+5/2)\sin^{n-2}\theta \\ &\qquad + (n-m-\tfrac{3}{2})\sin^n\theta] Y_l^{m+2} d\theta\end{aligned}$$

so that, using (9.3.6), we obtain

$$\int_0^\pi \sin^n\theta Y_l^m d\theta = \frac{m+\frac{1}{2}-n}{m+\frac{3}{2}+n}\left[\frac{(l-m-1)(l+m+2)}{(l-m)(l+m+1)}\right]^{\frac{1}{2}} \times \int_0^\pi \sin^n\theta Y_l^{m+2} d\theta. \quad (9.3.7)$$

Since in (9.3.5)

$$l-m = l_3-l_1+l_2 = \text{even number.}$$

(9.3.7) can be applied $(l_3-l_1+l_2)/2$ times and (9.3.5) is reduced to the known integral

$$\int_0^\pi \sin^{l_1+l_2+l_3+1}\theta d\theta.$$

Using (9.3.4), (9.3.7), and the value of the above integral we obtain, for $l_1=\alpha+\beta$,

$$\int_0^\pi \sin^{l_1}\theta Y_{l_2}^{\alpha} Y_{l_3}^{\beta} d\theta = \frac{(-1)^{(l_3-l_2-l_1)/2+\alpha}(2l_1)!!(l_3+l_2-l_1-1)!!}{(l_3+l_1-l_2)!!(l_2+l_1-l_3)!!(l_1+l_2+l_3+1)!!} \times \left[(2l_2+1)(2l_3+1)\frac{(l_3+\beta)!(l_2+\alpha)!}{(l_3-\beta)!(l_2-\alpha)!}\right]^{\frac{1}{2}} \quad (9.3.8)$$

where

$$(n)!! = n(n-2)(n-4)\cdots 2 \text{ or } 1, \quad (0)!! = (-1)!! = 1.$$

Combining (9.3.8) with (9.3.3) and the expression for $P_{l_1}^{l_1}$ leads finally to

$$\begin{aligned}\int_0^\pi &P_{l_1}^{m_1} Y_{l_2}^{m_2} Y_{l_3}^{m_3} d\theta \\ &= \frac{(l_3+l_2-l_1-1)!![(2l_1+1)(2l_2+1)(2l_3+1)]^{\frac{1}{2}}}{(l_3+l_1-l_2)!!(l_2+l_1-l_3)!!(l_1+l_2+l_3+1)!!} \times \left[\frac{(l_1+m_1)!(l_1-m_1)!(l_2-m_2)!(l_3-m_3)!}{2(l_2+m_2)!(l_3+m_3)!}\right]^{\frac{1}{2}} \\ &\times \sum_{i=0}^{l_1-m_1} \frac{(-1)^{(l_3-l_2+l_1)/2+m_3+i}(l_3+m_3+i)!(l_2+l_1-m_3-i)!}{(l_1-m_1-i)!(i)!(l_3-m_3-i)!(l_2-l_1+m_3+i)!}\end{aligned} \quad (9.3.9)$$

provided $m_1=m_2+m_3$.

In Elsasser's paper (15) there also appear expressions of the form

$$m_3 \int_0^\pi P_{l_1}^{m_1} \frac{d}{d\theta} P_{l_2}^{m_2} \cdot P_{l_3}^{m_3} d\theta - m_2 \int_0^\pi P_{l_1}^{m_1} P_{l_2}^{m_2} \frac{d}{d\theta} P_{l_3}^{m_3} d\theta, \quad m_1+m_2+m_3=0 \quad (9.3.10)$$

which can easily be reduced to the previous problem as follows: consider

$$\left\{m_2\cot\theta + \frac{d}{d\theta}\right\} P_{l_2}^{m_2} = [(l_2-m_2+1)(l_2+m_2)]^{\frac{1}{2}} P_{l_2}^{m_2-1}$$

$$\left\{m_3\cot\theta + \frac{d}{d\theta}\right\} P_{l_3}^{m_3} = [(l_3-m_3+1)(l_3+m_3)]^{\frac{1}{2}} P_{l_3}^{m_3-1}.$$

Multiplying these equations on the left by $m_3 P_{l_3}^{m_3}$ and $-m_2 P_{l_2}^{m_2}$ respectively and adding we obtain an expression which shows that (9.3.10) can be written in terms of two integrals of the form

$$\int_0^\pi P_{l_1}^{m_1-1} P_{l_2}^{m_2} P_{l_3}^{m_3} d\theta, \quad m_1 = m_2+m_3.$$

The argument used in (9.3.2) can be used again and, in fact, we would obtain exactly the same result (9.3.3) except that m_1 must be replaced by m_1-1 and the Y's by P's. Then, because the integrand contains P's rather than Y's, we require (9.3.8) with l_1 replaced by l_1-1.

The selection rules now require the l's to be equal to the sides of a triangle with odd perimeter. Also (9.3.10) is obviously zero if $m_2=m_3$ and $l_2=l_3$.

Finally it should be pointed out that the methods of this section can be used to evaluate any integral of the form

$$\int_0^\pi \sin^p\theta P_{l_1}^{m_1} P_{l_2}^{m_2}\cdots P_{l_n}^{m_n} d\theta$$

provided

$$\sum_{i=0}^{n} m^i - p + 1 = 0.$$

10. Type *B* Matrix Elements

10.1 Morse functions and diatomic molecules

Our next problem will be to evaluate

$$\int_{-\infty}^{\infty} x U_m^s U_{m'}^s dx.$$

U_m^s is defined by (5.1.4) so that, according to Sec. 5.2, the integral is proportional to the probability of a transition between two vibrational states of a diatomic molecule. The effect of the rotation is neglected.

As in 5.2 we can introduce the usual quantum numbers v, v' as follows

$$s-m=v, \quad s-m'=v'$$

so that our "intensity" integral is

$$I_{v,v'} = \int_{-\infty}^{\infty} x U_m^s U_{m'}^s dx. \tag{10.1.1}$$

Without loss of generality we can take $m'<m$ (or $v<v'$). This integral has been evaluated approximately for the first two bands ($v=0$, $v'=1, 2$) by Dunham (11).

Our calculation of (10.1.1) will fall into four parts and though the argument may seem lengthy we will find the same ideas being used in each part.

The first step is to show that

$$\int_{-\infty}^{\infty} U_m^{s-1} U_{m'}^s dx = 0, \quad m'<m. \tag{10.1.2}$$

Using (5.1.4) and Theorem II we obtain

$$\begin{aligned}
&\int_{-\infty}^{\infty} U_m^{s-1} U_{m'}^s dx \\
&\quad = [(s-m')(s+m')]^{-\frac{1}{2}} \\
&\qquad \times \int_{-\infty}^{\infty} U_m^{s-1} \left\{ \frac{\exp x}{2} - s - \frac{d}{dx} \right\} U_{m'}^{s-1} dx \\
&\quad = [(s-m')(s+m')]^{-\frac{1}{2}} \\
&\qquad \times \int_{-\infty}^{\infty} \left\{ \frac{\exp x}{2} - s + \frac{d}{dx} \right\} U_m^{s-1} \cdot U_{m'}^{s-1} dx.
\end{aligned} \tag{10.1.3}$$

Because of the orthogonality property satisfied by U_m^s we can replace s by $s-1$ inside the brackets. The operator will now operate on U_m^{s-1} so that

$$\begin{aligned}
&\int_{-\infty}^{\infty} U_m^{s-1} U_{m'}^s dx \\
&\quad = [(s-m')(s+m')]^{-\frac{1}{2}} [(s-m-1)(s+m-1)]^{\frac{1}{2}} \\
&\qquad \times \int_{-\infty}^{\infty} U_m^{s-2} U_{m'}^{s-1} dx.
\end{aligned}$$

If we apply this argument altogether $s-m$ times we obtain for the last stage, analogous to (10.1.3),

$$\begin{aligned}
&\int_{-\infty}^{\infty} U_m^{s-1} U_{m'}^s dx = [\text{constant}] \\
&\qquad \times \int_{-\infty}^{\infty} \left\{ \frac{\exp x}{2} - m - 1 + \frac{d}{dx} \right\} U_m^m \cdot U_{m'}^m dx
\end{aligned}$$

which vanishes because of the orthogonality and the definition of (5.1.4a). Thus (10.1.2) is proven.

The second part of our proof is to establish and use another reduction formula. We have

$$\begin{aligned}
I_{v,v'} &= [(s-m)(s+m)]^{-\frac{1}{2}} \\
&\quad \times \int_{-\infty}^{\infty} x \left\{ \frac{\exp x}{2} - s - \frac{d}{dx} \right\} U_m^{s-1} \cdot U_{m'}^s dx \\
&= [(s-m)(s+m)]^{-\frac{1}{2}} \\
&\quad \times \int_{-\infty}^{\infty} U_m^{s-1} \left\{ \frac{\exp x}{2} - s + \frac{d}{dx} \right\} x U_{m'}^s dx \\
&= [(s-m)(s+m)]^{-\frac{1}{2}} \\
&\quad \times \int_{-\infty}^{\infty} x U_m^{s-1} \left\{ \frac{\exp x}{2} - s + \frac{d}{dx} \right\} U_{m'}^s dx \\
&\quad + [(s-m)(s+m)]^{-\frac{1}{2}} \int_{-\infty}^{\infty} U_m^{s-1} U_{m'}^s dx.
\end{aligned}$$

The last integral vanishes because of (10.1.2) and we can use (5.1.4c) to obtain the reduction formula:

$$I_{v,v'} = \left[\frac{(s-m')(s+m')}{(s-m)(s+m)} \right]^{\frac{1}{2}} I_{v-1,v'-1}.$$

Applying this formula altogether $s-m=v$ times we obtain

$$\begin{aligned}
I_{vv'} &= \left[\frac{(s-m')!\Gamma(s+m'+1)\Gamma(2m+1)}{(s-m)!(m-m')!\Gamma(m+m'+1)\Gamma(s+m+1)} \right]^{\frac{1}{2}} \\
&\quad \times I_{0,v'-v}.
\end{aligned} \tag{10.1.4}$$

Furthermore, if we continue as above,

$$I_{0,\nu'-\nu}=[(m-m')(m+m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty} xU_m{}^m\left\{\frac{\exp x}{2}-m-\frac{d}{dx}\right\}U_{m'}{}^{m-1}dx$$
$$=[(m-m')(m+m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty} x\left\{\frac{\exp x}{2}-m+\frac{d}{dx}\right\}U_m{}^m\cdot U_{m'}{}^{m-1}dx$$
$$+[(m-m')(m+m')]^{-\frac{1}{2}}\int_{-\infty}^{\infty} U_m{}^mU_{m'}{}^{m-1}dx$$
$$=[(m-m')(m+m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty} U_m{}^mU_{m'}{}^{m-1}dx. \quad (10.1.5)$$

The first integral on the right side vanished because of the definition of (5.1.4a) and the remaining one can be evaluated by means of just one more recurrence formula.

This formula is obtained as follows:

$$\int_{-\infty}^{\infty} U_m{}^mU_{m'}{}^sdx$$
$$=[(s-m')(s+m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty} U_m{}^m\left\{\frac{\exp x}{2}-s-\frac{d}{dx}\right\}U_{m'}{}^{s-1}dx$$
$$=[(s-m')(s+m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty}\left\{\frac{\exp x}{2}-s+\frac{d}{dx}\right\}U_m{}^m\cdot U_{m'}{}^{s-1}dx$$
$$=[(s-m')(s+m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty}\left\{\frac{\exp x}{2}-m+\frac{d}{dx}\right\}U_m{}^m\cdot U_{m'}{}^{s-1}dx$$
$$+[(s-m')(s+m')]^{-\frac{1}{2}}(m-s)\int_{-\infty}^{\infty} U_m{}^mU_{m'}{}^{s-1}dx.$$

Again the first integral on the right side is zero because of the definition of (5.1.4a). We can now apply this reduction formula altogether $s-m'$ times to obtain (if $s<m$)

$$\int_{-\infty}^{\infty} U_m{}^mU_m{}^sdx =\left[\frac{\Gamma(2m'+1)}{(s-m')!\Gamma(s+m'+1)}\right]^{\frac{1}{2}}\frac{(m-m'-1)!}{(m-s-1)!} \times\int_{-\infty}^{\infty} U_m{}^mU_{m'}{}^{m'}dx. \quad (10.1.6)$$

But, because of (5.1.4a),

$$\int_{-\infty}^{\infty} U_m{}^mU_{m'}{}^{m'}dx=[\Gamma(2m)\Gamma(2m')]^{-\frac{1}{2}} \times\int_{-\infty}^{\infty}\exp[(m+m')x-\exp x]dx$$
$$=[\Gamma(2m)\Gamma(2m')]^{\frac{1}{2}}\Gamma(m+m'). \quad (10.1.7)$$

Collecting the results (10.1.4–7) we finally obtain the required formula

$$I_{\nu,\nu'}=\frac{2}{(m-m')(m+m')}\left[\frac{(s-m')!\Gamma(s+m'+1)}{(s-m)!\Gamma(s+m+1)}mm'\right]^{\frac{1}{2}}.$$

If we put $m=s-\nu$, $m'=s-\nu'$ so that the final result is in terms of the physical constant s (see 5.2) and the quantum numbers ν, ν', we obtain, for $\nu<\nu'$,

$$I_{\nu,\nu'}=\frac{2}{(\nu'-\nu)(2s-\nu-\nu')} \times\left[\frac{\nu'!\Gamma(2s-\nu'+1)}{\nu!\Gamma(2s-\nu+1)}(s-\nu)(s-\nu')\right]^{\frac{1}{2}}. \quad (10.1.8)$$

11. Type *D* Matrix Elements

11.1 Harmonic oscillator

From the recurrence relations (6.1.4) for the harmonic oscillator eigenfunctions we obtain immediately

$$\xi\psi_N=[(N+1)/2]^{\frac{1}{2}}\psi_{N+1}+[N/2]^{\frac{1}{2}}\psi_{N-1}.$$

Since the ψ's are orthonormal this formula enables us to calculate the transition probabilities. In fact

$$\int_{-\infty}^{\infty}\psi_{N'}\xi\psi_N d\xi=\begin{cases}[(N+1)/2]^{\frac{1}{2}} & \text{if } N'=N+1\\ [N/2]^{\frac{1}{2}} & \text{if } N'=N-1\\ 0 & \text{otherwise.}\end{cases}$$

Similarly the momentum matrix elements can be found from

$$\frac{d}{d\xi}\psi_N=-\left[\frac{N+1}{2}\right]^{\frac{1}{2}}\psi_{N+1}\left[\frac{N}{2}\right]^{\frac{1}{2}}\psi_{N-1}.$$

The recurrence relations (6.1.4) were used in this manner to find the matrix elements even before they were used to generate the solutions themselves (see, for example, 9, p. 135).

12. Type *F* Matrix Elements

For the purpose of discussion we shall consider the Schrödinger hydrogen intensity integral

$$I_{n',n}{}^{l-1,l}=\int_0^{\infty} rR_{n'}{}^{l-1}R_n{}^l dr$$

where R is defined by (8.1.5). The value of this integral has been calculated many times. Originally Schrödinger (40, p. 99) calculated it for special cases using the generating function for Laguerre polynomials. Wheeler (52) has recently applied this method to the general case of discrete-discrete transitions. Epstein (16) used the theory of hypergeometric functions to solve the same problem while Eckart (13) evaluated the integral directly. Gordon (19) has treated the discrete-continuous and continuous-continuous as well as the discrete-discrete transitions.

We want to show that each of the $\mathfrak{K}$ and O operator recurrence formulas of Chapter 8 for the radial functions leads to a recurrence formula for the integral itself, provided that at least one of the wave functions represents a bound electron. The O-operator method will then be generalized so that the more complicated Dirac matrix elements can be calculated.

12.1 Algebraic recurrence formulas for intensities

It is not difficult to verify from (8.1.5) and (8.1.6) that

$$2lA_{n'}{}^{l}+\mathfrak{K}_{n'}{}^{l}=(2l+1)A_{n}{}^{l+1}+\mathfrak{K}_{n}{}^{l+1}$$
$$+A_{n'}{}^{l+1}-\mathfrak{K}_{n'}{}^{l+1}+\text{constant}/r. \quad (12.1.1)$$

Multiplying (12.1.1) on the left by $rR_n{}^l$, on the right by $R_{n'}{}^l$, and integrating gives

$$\begin{aligned}2lA_{n'}{}^{l}&\int_0^\infty rR_n{}^{l}+\mathfrak{K}_{n'}{}^{l}R_{n'}{}^{l}dr\\ &=(2l+1)A_{n}{}^{l+1}\int_0^\infty rR_n{}^{l}+\mathfrak{K}_{n}{}^{l+1}R_{n'}{}^{l}dr\\ &\qquad+A_{n'}{}^{l+1}\int_0^\infty rR_n{}^{l}-\mathfrak{K}_{n'}{}^{l+1}R_{n'}{}^{l}dr\\ &=(2l+1)A_{n}{}^{l+1}\int_0^\infty r(-\mathfrak{K}_{n}{}^{l+1}R_{n}{}^{l})R_{n'}{}^{l}dr\\ &\qquad+A_{n'}{}^{l+1}\int_0^\infty rR_n{}^{l}-\mathfrak{K}_{n'}{}^{l+1}R_{n'}{}^{l}dr\end{aligned}$$

because $R_n{}^l$, $R_{n'}{}^l$ are orthogonal and their product vanishes at $r=0,\ \infty$. We have then:

$$\left.\begin{aligned}&2lA_{n'}{}^{l}\,I_{n',\,n}{}^{l-1,l}=(2l+1)A_{n}{}^{l+1}\,I_{n',\,n}{}^{l,l+1}\\ &\qquad\qquad+A_{n'}{}^{l+1}\,I_{n',\,n}{}^{l+1,l}.\\ &\text{By interchanging } n, n' \text{ we obtain}\\ &2lA_{n}{}^{l}\,I_{n',\,n}{}^{l,l-1}=A_{n}{}^{l+1}\,I_{n',\,n}{}^{l,l+1}\\ &\qquad\qquad+(2l+1)A_{n'}{}^{l+1}\,I_{n',\,n}{}^{l+1,l}\\ &\text{where}\\ &\qquad A_n{}^{l}=[(n-l)(n+l)]^{\frac{1}{2}}/nl.\end{aligned}\right\} \quad (12.1.2)$$

Our derivation (and hence this result) is valid for the discrete-continuous transitions once one replaces n by in.

These are algebraic formulas giving a pair of intensities in terms of the next highest pair in the scheme of Fig. 3.

All intensities can now be calculated once a starting point is found; an obvious choice is the pair at the top of the n' ladder:

$$I_{n',\,n}{}^{n',n'-1} \quad \text{and} \quad I_{n',\,n}{}^{n'-1,n'}$$

where

$$I_{n',\,n}{}^{n',n'-1}=0. \quad (12.1.3a)$$

(We shall adopt the convention that n' always refers to the discrete spectrum.) The method of calculation of the other expression is indicated in 12.4. The result is:

$$I_{n',\,n}{}^{n'-1,n'}=2^{2n'+2}(nn')^{n'+2}$$
$$\times\left[\frac{(n+n')!}{(n-n'-1)!(2n'-1)!}\right]^{\frac{1}{2}}\frac{(n-n')^{n-n'-2}}{(n+n')^{n+n'+2}} \quad (12.1.3b)$$

or, for the discrete-continuous transition,

$$I_{n',\,in}{}^{n'-1,n'}=2^{2n'+2}(nn')^{n'+2}$$
$$\times\left[\frac{n^3\prod_{p=1}^{n'}(p^2+n^2)}{(2n'-1)!\,(\exp(2n\pi)-1)}\right]^{\frac{1}{2}}$$
$$\times\frac{\exp[2n\tan^{-1}(n/n')]}{(n^2+n'^2)^{n'+2}}. \quad (12.1.3c)$$

From (12.1.3) we can now calculate pairs of intensities by successive application of (12.1.2)—the important intensities requiring at most but a few steps.

12.2 Operator recurrence formula for intensities

The results of 8.2 will now be used to find an n'-changing recurrence relation for the intensities. Indeed, it follows immediately from (8.2.3) that

$$\left.\begin{aligned}&I_{n'+1,\,n}{}^{l-1,l}(s)=O_{n'+1}{}^{l-1}I_{n',\,n}{}^{l-1,l}(s)\\ &\text{or}\\ &I_{n'+1,\,in}{}^{l-1,l}(s)=O_{n'+1}{}^{l-1}I_{n',\,in}{}^{l-1,l}(s)\\ &\text{with}\\ &O_{n'+1}{}^{l-1}=\frac{n'^{l+1}}{(n'+1)^{l+1}(2n'+1)}\left[\frac{n'+l}{n'-l+1}\right]^{\frac{1}{2}}\\ &\qquad\times\left\{2n'+1+(s+1/n')\frac{d}{ds}\right\}\end{aligned}\right\} \quad (12.2.1)$$

where the intensity *function* is defined by

$$I_{n',n}{}^{l-1,l}(s)=\int_0^\infty rR_{n'}{}^{l-1}(s)R_n{}^l dr.$$

The starting point needed here is

$$I_{l,n}{}^{l-1,l}(s)=\frac{1}{n}\left(\frac{4}{nl}\right)^{l+1}\left[\frac{(n+l)!}{(n-l-1)!(2l-1)!}\right]^{\frac{1}{2}}\times\frac{(s-1/n)^{n-l-2}}{(s+1/n)^{n+l+2}}[(l+1)s-1] \quad (12.2.2a)$$

or

$$I_{l,in}{}^{l-1,l}(s)=\left(\frac{4}{nl}\right)^{l+1}\left[\frac{n\prod_{p=1}^{l}(p^2+n^2)}{(2l-1)!(\exp(2n\pi)-1)}\right]^{\frac{1}{2}}\times\frac{\exp(2n\tan^{-1}ns)}{(s^2+1/n^2)^{l+2}}[(l+1)s-1]. \quad (12.2.2b)$$

The derivation of (12.2.2) is indicated in 12.4. Another starting point which may be needed is

$$I_{l+1,in}{}^{l,l-1}(s).$$

It is slightly more complicated but can be found easily from the formulas in 12.4.

Using (12.2.1) and (12.2.2a) we can find

$$I_{l+1,n}{}^{l-1,l}(s),\ \cdots,\ I_{n',n}{}^{l-1,l}(s)$$

which, with (8.2.2), give the intensities. Similarly, from (12.2.2b) we can find

$$\cdots,\ I_{n',in}{}^{l-1,l}(s).$$

12.3 Remarks on 12.1 and 12.2

(1) The set of values of the quantum numbers for which the intensities are required will determine which of the above two methods should be used. Being algebraic (12.1.2) is simpler whereas (12.2.1) has the special characteristic that it is applicable to the problem of calculating more general matrix components:

$$\int_0^\infty V(r)R_{n'}{}^{l'}R_n{}^l dr.$$

This fact is essential to the treatment of Dirac matrix elements in a later section.

(2) Example of a calculation:

To find

$$I_{2,n}{}^{0,1}=\int_0^\infty rR_2{}^0R_n{}^1 dr$$

we can use (12.1.3b) to get immediately

$$I_{2,n}{}^{2,1}=0$$

$$I_{2,n}{}^{1,2}=3^{-1/2}2^{19/2}n^{9/2}(n^2-1)^{1/2}(n-2)^{n-7/2}(n+2)^{-n-7/2}.$$

From (12.1.2):

$$I_{2,n}{}^{0,1}=(1/2A_2{}^1)3A_n{}^2I_{2,n}{}^{1,2}+0$$
$$=2^{17/2}n^{7/2}(n^2-1)^{1/2}(n-2)^{n-3}(n+2)^{-n-3}.$$

Alternatively, we can use (12.2.2a) to get

$$I_{1,n}{}^{0,1}(s)=2^4n^{-5/2}(n^2-1)^{1/2}\times(s-1/n)^{n-3}(s+1/n)^{-n-3}(2s-1).$$

Operating on this expression with

$$O_2{}^0=2^{-3/2}3^{-1}\left\{3+(1+s)\frac{d}{ds}\right\}$$

and then putting $s=\frac{1}{2}$ we get the value above for $I_{2,n}{}^{0,1}$ which is the same as that given by Condon and Shortley (5) for the transition $2s-np$.

(3) The above methods can lead to *explicit forms* of the intensity integral except in the case of continuous-continuous transitions. For example, by means of (12.1.2), (12.1.3), and known relations between contiguous hypergeometric functions the results given by Gordon (19) can be proven by induction.

12.4 Certain integrals and the problem of normalization

We have yet to show how the starting points given in 12.1 and 12.2 are found. To this purpose we define

$$I_n=\int_0^\infty r^l\exp(-sr)R_n{}^l dr \quad (12.4.1)$$

and we must distinguish between two cases:

Case I: Discrete-discrete.—From (8.1.3) and (8.1.4)

$$\int_0^\infty r^{l+1}\exp(-sr)\left\{\frac{d^2R}{dr^2}+\frac{2}{r}R-\frac{l(l+1)}{r^2}R-\frac{1}{n^2}R\right\}dr=0.$$

After two partial integrations of the first term we obtain

$$(s^2-1/n^2)\frac{dI_n}{ds}+[2(l+1)s-2]I_n=0.$$

Therefore

$$I_n=C\frac{(s-1/n)^{n-l-1}}{(s+1/n)^{n+l+1}}.$$

I_n is the Laplace transform of $r^lR_n{}^l$ and therefore (4, p. 170)

$$R_n{}^l=r^{-l}[\text{residue of }\{\exp(sr)I_n\}\text{ at }s=-1/n].$$

The coefficient of the lowest power $(l+1)$ of r turns out to be

$$C\exp(-r/n)/(2l+1)!. \quad (12.4.2)$$

But from (8.1.5) we have:

$$R_n{}^l=+\mathfrak{C}_n{}^{l+1}+\mathfrak{C}_n{}^{l+2}\ldots+\mathfrak{C}_n{}^{n-1}R_n{}^{n-1}.$$

Using (8.1.5a) and (8.1.6) we can easily pick out the coefficient of r^{l+1}; it is

$$\frac{2^n(n-1)!}{n^{l+2}(2n-1)!l!}\left[\frac{(n+l)!}{(n-l-1)!}\right]^{\frac{1}{2}} \times[(2l+3)(2l+5)\cdots(2n-1)]\exp(-r/n). \quad (12.4.3)$$

Equating (12.4.2) and (12.4.3) we find C so that

$$I_n=\frac{2^{l+1}}{n^{l+2}}\left[\frac{(n+l)!}{(n-l-1)!}\right]^{\frac{1}{2}}\frac{(s-1/n)^{n-l-1}}{(s+1/n)^{n+l+1}}. \quad (12.4.4)$$

Then

$$I_{l,n}{}^{l-1,l}(s)=(2/l)^{l+\frac{1}{2}}[(2l)!]^{-\frac{1}{2}}\int_0^\infty r^{l+1}\exp(-sr)R_n{}^l dr$$

$$=(2/l)^{l+\frac{1}{2}}[(2l)!]^{-\frac{1}{2}}\left[-\frac{dI_n}{ds}\right].$$

Therefore

$$I_{l,n}{}^{l-1,l}(s)=\frac{1}{n}\left(\frac{4}{nl}\right)^{l+1}\left[\frac{(n+l)!}{(n-l-1)!(2l-1)!}\right]^{\frac{1}{2}} \times\frac{(s-1/n)^{n-l-2}}{(s+1/n)^{n+l+2}}[(l+1)s-1]. \quad (12.2.2a)$$

By putting $l=n'$ and $s=1/n'$, we obtain

$$I_{n',n}{}^{n'-1,n'}=2^{2n'+2}(nn')^{n'+2} \times\left[\frac{(n+n')!}{(n-n'-1)!(2n'-1)!}\right]^{\frac{1}{2}}\frac{(n-n')^{n-n'-2}}{(n+n')^{n+n'+2}}. \quad (12.1.3b)$$

Case II: Discrete-continuous.—In this case I_{in} turns out to be

$$I_{in}=C(s-i/n)^{-in-l-1}(s+i/n)^{in-l-1}$$

$$=C\frac{\exp(2n\tan^{-1}ns-n\pi)}{(s^2+1/n^2)^{l+1}},\quad 0<\tan^{-1}ns<\pi/2 \quad (12.4.5)$$

and the inverse transform is

$$R_{in}{}^l=\frac{Cr^{-l}}{2\pi i}\int\exp(sr)(s-i/n)^{-in-l-1} \times(s+i/n)^{in-l-1}ds \quad (12.4.6)$$

where the contour can be taken as shown in Fig. 5. This is the form in which the positive energy radial function was originally given by Schrödinger (39). The normalization condition can be written as (2, p. 291).

$$\lim_{\Delta k\to 0}\int_0^\infty R_{in}{}^l\left\{\int_{k-\Delta k}^{k+\Delta k}R_{in}{}^l dk\right\}dr=1,\quad k=1/n.$$

There is no contribution to this limit for finite values of r. We can therefore substitute the asymptotic form of $R_{in}{}^l$. This is found by expanding the integrand of (12.4.6) in descending powers of r on each half of the contour. The first terms in each expansion are conjugate complex and their sum turns out to be

$$R_{in}{}^l\sim\frac{C\exp(-n\pi/2)n^{l+1}}{|\Gamma(l+1-in)|2^l} \times\cos(r/n+n\log(2r/n)-(l+1)\pi/2+\sigma_l)$$

where σ_l is the argument of $\Gamma(l+1-in)$.

Using the normalization condition, we obtain the value of C and finally,

$$I_{in}=\left(\frac{2}{n}\right)^{l+\frac{1}{2}}\left[\frac{2\prod_{p=1}^{l}(p^2+n^2)}{\exp(2n\pi)-1}\right]^{\frac{1}{2}}\frac{\exp(2n\tan^{-1}ns)}{(s^2+1/n^2)^{l+1}} \quad (12.4.7)$$

from which the corresponding starting points are found to be as in (12.1.3c) and (12.2.2b).

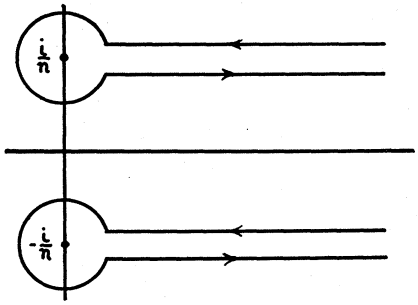


FIG. 5. Contour in the s-plane for the positive energy solutions (12.4.6) of the Kepler problem.

12.5 Generalization to Dirac matrix elements

We want now to find the formulas which are needed in the calculation of matrix elements which contain Dirac radial functions in their integrands. In Sec. 8.4 we found that these functions are linear combinations of the generalized Kepler functions in 8.3. Dirac matrix elements are therefore linear combinations of integrals such as

$$\int_0^\infty V(r)R_{n'+\gamma'}{}^{l'+\gamma'}(a'r)R_{n+\gamma}{}^{l+\gamma}(ar)dr \quad (12.5.1a)$$

$$\int_0^\infty V(r)R_{n'+\gamma'}{}^{l'+\gamma'}(a'r)R_{in+i\gamma}{}^{l+\gamma}(ar)dr \quad (12.5.1b)$$

where $V(r)$ is the perturbing potential and $l, l'=0, -1$. The generalized O-operator recurrence relation (8.3.2b, c) enables us to raise n' in these integrals and does not depend on the form of $V(r)$. Our problem is

therefore reduced to that of finding expressions for the starting functions corresponding to I_n, I_{in} of the previous section.

If we consider

$$V(r)=r^p \exp(-qr),$$

where p, q are constants,[11] all that remains is to find

$$I_{n+\gamma}(t,u)=\int_0^\infty x^t \exp(-ux)R_{n+\gamma}{}^{l+\gamma}(x)dx,$$

$$x=ar \quad (12.5.2a)$$

$$I_{in+i\gamma}(t,u)=\int_0^\infty x^t \exp(-ux)R_{in+i\gamma}{}^{l+\gamma}(x)dx \quad (12.5.2b)$$

and later put $t=p+\gamma'$ or $p+\gamma'+1$ and $u=q/a+sa'/a$.

The new feature is that the differential equation for I is no longer of the first order. Instead, proceeding as in 12.4 we obtain:

Case I: Discrete-discrete.—

$$[u^2-1/(n+\gamma)^2]\frac{d^2I}{du^2}+[(2+t)2u-2]\frac{dI}{du}$$
$$+(1+t-l-\gamma)(2+t+l+\gamma)I=0.$$

The general solution of this equation, convergent for large u, is

$$I_{n+\gamma}(t,u)=A[2/(un+u\gamma+1)]^{2+t+l+\gamma}$$
$$\times F(2+t+l+\gamma,\ 1+l-n,\ 2+2l+2\gamma,\ 2/(un+u\gamma+1))$$
$$+B[2/(un+u\gamma+1)]^{1+t-l-\gamma}$$
$$\times F(1+t-l-\gamma,\ -n-l-2\gamma,\ -2l-2\gamma,\ 2/(un+u\gamma+1)). \quad (12.5.3)$$

Taking the inverse transform term by term it is found that $B=0$ if R is to satisfy the boundary condition. Then comparing coefficients exactly as was done in 12.4, it turns out that A is such that

$$I_{n+\gamma}(t,u)=\left(\frac{n+\gamma}{2}\right)^t(l+\gamma+1)\frac{\Gamma(2+t+l+\gamma)}{\Gamma(2l+2\gamma+3)}$$
$$\times\left[\frac{\Gamma(n+l+2\gamma+1)}{(n-l-1)!}\right]^{\frac{1}{2}}[2/(un+u\gamma+1)]^{2+t+l+\gamma}$$
$$\times F(2+t+l+\gamma,\ 1+l-n,\ 2+2l+2\gamma,\ 2/(un+u\gamma+1)). \quad (12.5.4a)$$

Case II: Discrete-continuous.—It is convenient to use here the notation and some results given by Whittaker and Watson (53, Chapter XVI) so that replacing $n+\gamma$ by $in+i\gamma$ in (12.5.3) (with $B=0$) and taking the inverse transform term by term we obtain

$$R_{in+i\gamma}{}^{l+\gamma}(x)=\frac{A2^{t+1}\exp[-(t+1)i\pi/2]}{\Gamma(2+t+l+\gamma)(n+\gamma)^{t+1}}M_{in+i\gamma,\,l+\gamma+\frac{1}{2}}(-2ix/(n+\gamma))$$
$$\sim\frac{A2^{t+1}\Gamma(2l+2\gamma+2)\exp[-(n+\gamma)\pi/2-i(t+l+\gamma+2)\pi/2]}{(n+\gamma)^{t+1}|\,\Gamma(l+\gamma+1-in-i\gamma)\,|\,\Gamma(2+t+l+\gamma)}$$
$$\times 2\cos(x/(n+\gamma)+(n+\gamma)\log(2x/(n+\gamma))-(l+\gamma+1)\pi/2-\sigma)$$

where $\sigma=\arg\Gamma(l+\gamma+1+in+i\gamma)$. Normalizing as in 12.4 leads to a value of A so that

$$I_{in+i\gamma}(t,u)=\left(\frac{n+\gamma}{2}\right)^{t+1}\frac{\Gamma(2+t+l+\gamma)}{\Gamma(2l+2\gamma+2)}$$
$$\times\left[\frac{(n+\gamma)\prod_{p=1}^{l}((p+\gamma)^2+(n+\gamma)^2)}{\exp(2n\pi+2\gamma\pi)-1}\right]^{\frac{1}{2}}$$
$$\times\frac{\exp[i(t+l+\gamma+2)\pi/2+(n+\gamma)\pi]}{[(iun+iu\gamma+1)/2]^{2+t+l+\gamma}}$$
$$\times F(2+t+l+\gamma,\ 1+l+\gamma-in-i\gamma,$$
$$2+2l+2\gamma,\ 2/(iun+iu\gamma+1)). \quad (12.5.4b)$$

Equations (12.5.4) provide the starting points for the matrix elements of generalized Kepler functions once we replace t by $p+\gamma'$ or $p+\gamma'+1$ and u by $q/a+sa'/a$.

Finally we can find the solutions of Dirac's equations for energies greater than E_0. As stated earlier, this amounts to replacing $n+\gamma$ by $in+i\gamma$ in (8.4.4) and showing that (8.4.7) is the proper value of the normalization constant C.

Let us take the normalization condition to be

$$\lim_{\Delta k\to 0} a^{-1}\int_0^\infty \chi_1\left[\int_{k-\Delta k}^{k+\Delta k}\chi_1 dk\right]dx$$
$$+\lim_{\Delta k\to 0} a^{-1}\int_0^\infty \chi_2\left[\int_{k-\Delta k}^{k+\Delta k}\chi_2 dk\right]dx=1$$

with $k=1/(n+\gamma)$. We need only the asymptotic expansions of the wave functions and they can be written

[11] This potential is general enough to include all integrals considered, for example, by Hulme (23) in calculating the relativistic internal conversion coefficient for radium C.

in terms of the asymptotic forms found in this section for the normalized R's. That is, in terms of

$$R_{in+i\gamma}{}^{l+\gamma}(x)\sim(2/\pi)^{\frac{1}{2}}\cos(x/(n+\gamma)+(n+\gamma)\log(2x/(n+\gamma))+(l+\gamma+1)\pi/2-\sigma).$$

We obtain

$$\chi_1\sim 2\gamma C(2(\epsilon-1)/\pi)^{\frac{1}{2}}\cos(x/(n+\gamma)+(n+\gamma)\log(2x/(n+\gamma))-\sigma_1)$$
$$\chi_2\sim 2\gamma C(2(\epsilon+1)/\pi)^{\frac{1}{2}}\cos(x/(n+\gamma)+(n+\gamma)\log(2x/(n+\gamma))-\sigma_2)$$

where σ_1, σ_2, are unimportant phase factors. The integrals over the cosine terms are as before and the normalization condition leads finally to the value

$$C=(a/2\epsilon)^{\frac{1}{2}}/2\gamma. \tag{8.4.7}$$

Thus, to find a Dirac matrix element, we use (8.4.4) with the appropriate C to express the required integral as a linear combination of integrals like (12.5.1). These integrals can be derived from (12.5.2, 4) by means of the O-operator (8.3.2b, c) and the definition (8.3.1a). The result will be a linear combination of hypergeometric functions. As explained after Eqs. (4.9.7), this combination can be reduced finally to at most two[12] hypergeometric functions before computations have to be made.

It is customary to normalize the eigenfunctions with respect to *energy* by writing the eigendifferentials as

$$\int_E^{E+\Delta E}\chi dE/\hbar.$$

This normalization leads (18) to the following physical interpretation of the wave functions: they represent a stream of electrons with energy E crossing a large sphere about the center of force and there is one encounter per unit time. The transition probabilities would then be proportional to the number of electrons observed per unit energy range. *Our* normalization is consistent with that given for the ordinary Kepler problem and is with respect to *velocity* so that the transition probabilities are proportional to the number of electrons observed per unit velocity range. To change from our normalization to the more usual we merely multiply the wave functions by

$$\left[\frac{\mu c^2}{\hbar}\frac{d\epsilon}{dk}\right]^{-\frac{1}{2}}=[(n+\gamma)\hbar/\epsilon\mu]^{\frac{1}{2}}/c\alpha Z\epsilon.$$

13. Approximation Procedure

We shall now indicate how the methods of Chapters 2 and 3 can be generalized to handle perturbation problems.

The idea is simply the following: we try to satisfy the fundamental differential-difference equation (3.1.2) up to a given order in a small parameter ϵ, with the substitutions

$$k(x,m)={}^{(0)}k(x,m)+\epsilon\,{}^{(1)}k(x,m)+\epsilon^2\,{}^{(2)}k(x,m)+\cdots$$
$$L(m)={}^{(0)}L(m)+\epsilon\,{}^{(1)}L(m)+\epsilon^2\,{}^{(2)}L(m)+\cdots.$$

When these functions are found they enable us to calculate, through (3.1.1), the corresponding perturbed potential function.

$$r(x,m)={}^{(0)}r(x,m)+\epsilon\,{}^{(1)}r(x,m)+\epsilon^2\,{}^{(2)}r(x,m)+\cdots.$$

A table of k, L, and r functions would then enable us to handle perturbed problems exactly as we handled unperturbed problems in earlier chapters.

If the above procedure is carried out the zero-order approximation will lead to exactly the types $A\cdots F$. The first-order approximation requires further that

$$2\,{}^{(0)}k(x,m+1)\,{}^{(1)}k(x,m+1)-2\,{}^{(0)}k(x,m)\,{}^{(1)}k(x,m)+{}^{(1)}k'(x,m+1)+{}^{(1)}k'(x,m)={}^{(1)}L(m)-{}^{(1)}L(m+1) \tag{13.0.1}$$

where the prime ($'$) denotes differentiation with respect to x. This equation would now have to be solved for the ${}^{(1)}k$ and ${}^{(1)}L$ functions belonging to each ${}^{(0)}k$ and ${}^{(0)}L$. Unlike the equation for the zero-order approximation however, our new equation is *linear* in the unknown functions; we therefore find that there is no restriction on s in the trial solution

$${}^{(1)}k(x,m)=\sum_{i=-t}^{s}k_i m^i,\quad k_i\equiv{}^{(1)}k_i(x). \tag{13.0.2}$$

Each of the types $A\cdots F$, then, generates an *infinite number* of perturbation problems which can be factorized.

The second-order approximation requires that the following linear equation for ${}^{(2)}k$, ${}^{(2)}L$ be satisfied

$${}^{(1)}k^2(x,m+1)+2\,{}^{(0)}k(x,m+1)\,{}^{(2)}k(x,m+1)-{}^{(1)}k^2(x,m)-2\,{}^{(0)}k(x,m)\,{}^{(2)}k(x,m)+{}^{(2)}k'(x,m+1)+{}^{(2)}k'(x,m)={}^{(2)}L(m)-{}^{(2)}L(m+1) \tag{13.0.3}$$

and so on for higher order approximations.

The ideas used in solving these new differential-difference equations are the same as those used in Chapter 3 but it is easily seen that the actual calculations become much more complex as the order and complexity of the perturbation increases. We must therefore consider what circumstances would make the above procedure preferrable to standard approximation procedures.

Standard methods lead to expressions for the corrections to the eigenvalues and eigenfunctions in terms of matrix elements, and the formulas developed in Chapters 9–12 could then be used to evaluate these corrections. The formulas of Chapter 12 are, however, much more complicated than those of 9–11. We might therefore expect to find our new method most suitable for calculating perturbations to type F problems. This *is*

[12] To obtain series which converge rapidly it may be necessary to introduce a transformation which doubles this number (see 23).

the case, and so we shall work out in detail the Stark effect problem in Sec. 13.2.

The new method has also been checked in detail with the known results for type A (rotating polar molecule in an electric field) and type C (anharmonic oscillator) problems; but the factorization method is the more complicated in these cases, at least up to the order of approximation (second) which was considered.

Besides the advantage of the new method with type F problems, there are two other reasons why, in some cases, it would be preferred even for type $A\cdots E$ problems. In the first place, we do not require any knowledge of the perturbed eigenfunction for one order of approximation before finding the eigenvalues to the next order; we simply write down the eigenvalues in terms of ${}^{(0)}L$, ${}^{(1)}L$, ${}^{(2)}L$, $\cdots$. Secondly, our perturbed eigenfunctions are not given in the form of expansions in terms of the unperturbed eigenfunctions; they can be derived quickly from a key function which is a *closed* expression and which is *easily normalized.*

13.1 Type F perturbations

We now consider perturbations to type F problems. That is, we take

$$ {}^{(0)}k(x, m)=m/x+q/m. \tag{13.1.1}$$

We will purposely find a perturbed factorization (to the first order) which is much more general than necessary for the Stark effect problem. This will enable us to understand better the general features of the method. We shall then specialize the results for the second-order calculations and finally, in the next section, apply them to the Stark effect problem.

Using the above expression for ${}^{(0)}k(x, m)$ let us substitute (13.0.2) into (13.0.1); we want to find what k_i satisfy the resulting equation. We need to merely sketch the first step in the solution: the left side of our equation must be a function of m only; therefore, if we multiply through by $(m+1)^{i+1}$ and consider the left side arranged in powers of m, we know that the coefficient of each power must be a constant. Similarly the left side can be arranged in powers of $(m+1)$ after multiplying through by m^{i+1} and the resulting coefficients of each power must also be constants. If the coefficients of the negative powers in each of these cases are equated to constants it will easily be seen that

$$k_i=0 \quad \text{for} \quad i<-2$$

and k_{-2}, k_{-1} must be constants.

This simplification enables us to solve (13.0.1) for ${}^{(1)}L(m)$; but we must first find the anti-difference of

$$ {}^{(1)}k'(x, m+1)+{}^{(1)}k'(x, m)=\sum_{i=0}^{s} k_i'[(m+1)^i+m^i]$$

$$\equiv\sum_{i=0}^{s} k_i'[f_i(m+1)-f_i(m)],$$

say. That is, we want to find $f_i(m)$.

Although a general formula for $f_i(m)$ can be found we need to know only two facts about $f_i(m)$. First, $f_i(m)$ is obviously a series of positive powers of m with the highest power $(i+1)$. Second, the powers are either all even or all odd; this can be seen by comparing

$$(m+1)^i+m^i=f_i(m+1)-f_i(m)$$

with the result obtained by replacing (m) by $(-m-1)$ in this equation; that is, with

$$(-m)^i+(-m-1)^i=f_i(-m)-f_i(-m-1).$$

We obtain

$$\begin{aligned} f_i(-m-1)-f_i(-m)&=(-1)^{i+1}[(m+1)^i+m^i]\\ &=(-1)^{i+1}[f_i(m+1)-f_i(m)].\end{aligned}$$

If we neglect the fact (which anyway is not important for our discussion) that $f_i(m)$ is determined only to within an arbitrary function of x and m of period one in m, we can conclude that

$$f_i(-m)=(-1)^{i+1}f_i(m).$$

Thus $f_i(m)$ contains only even powers of m if i is odd and only odd powers if i is even.

From (13.0.1) we now obtain

$$ {}^{(1)}L(m)=-2\ {}^{(0)}k(x, m)\ {}^{(1)}k(x, m)-\sum_{i=0}^{s} k_i'f_i(m)$$

where the first term on the right side is given by (13.1.1) and (13.0.2). If we now substitute

$$ {}^{(1)}L(m)=-\sum_{i=-3}^{s+1}\alpha_i m^i, \quad \alpha_i=\text{constant}$$

and equate the coefficients of like powers of m on either side we are led to a system of first-order differential equations for the k_i.

The first three equations are

$$\begin{aligned} 2qk_{-2}&=\alpha_{-3}\\ 2qk_{-1}&=\alpha_{-2}\\ 2qk_0+2k_{-2}/x&=\alpha_{-1}.\end{aligned}$$

As in Chapter 3 the equation containing α_0 contributes nothing and we can take $\alpha_0=0$ without loss of generality. The remaining equations are of the form

$$\begin{aligned} 2k_i/x+2qk_{i+2}+2k_i'/(i+1)+(\ )k_{i+2}'\\ +(\ )k_{i+4}'+\cdots=\alpha_{i+1}, \quad i=0, 1, \cdots s\end{aligned}$$

where the brackets contain constants which depend on the coefficients in $f_i(m)$. The last two equations are simply

$$\begin{aligned} 2k_{s-1}/x+2k_{s-1}'/s&=\alpha_s\\ 2k_s/x+2k_s'/(s+1)&=\alpha_{s+1}.\end{aligned}$$

Before actually solving a particular system of the equations we can show that

$$\left.\begin{aligned} &k_{-2}=k_0=k_2=\cdots=0\\ \text{and therefore}\quad &\\ &\alpha_{-3}=\alpha_{-1}=\alpha_1=\cdots=0.\end{aligned}\right\} \tag{13.1.2}$$

This result is not surprising when we note that the k_i with odd i are determined by equations whose number is the same as the number of such k_i whereas the k_i with even i must satisfy one more equation than the number of such k_i. To prove our result let us consider s to be even. Then, from the last equation,

$$k_s=(s+1)\alpha_{s+1}x/2(s+2)+C_{s+1}/x^{s+1}$$

where C_i will denote the constant of integration in the equation containing α_i. (If s is odd we merely solve the second last equation and proceed as in the following argument.) Then, considering the equations containing α_{s-1}, α_{s-3}, $\cdots$ we can find the form of k_{s-2}, k_{s-4}, $\cdots$ in turn. It is not difficult to find eventually that k_0 contains terms only of the form

$$1/x^{s+1},\ 1/x^s,\ \cdots 1/x^2,\ x,\ x^2,\ x^3,\ \cdots.$$

But this result cannot be reconciled with the first and third equations unless (13.1.2) is satisfied.

Let us now find the complete solution for a special case. Let us take $s=3$; our differential equations then become

$$\begin{aligned}&2qk_{-1}=\alpha_{-2}\\&2k_1/x+k_1'+2qk_3+k_3'/2=\alpha_2\\&2k_3/x+k_3'/2=\alpha_4.\end{aligned}$$

The general solutions of these equations lead to

$$\begin{aligned}{}^{(1)}k(x,m)&=\alpha_{-2}/2qm+[(\alpha_2/3-\alpha_4/15)x\\&\quad-q\alpha_4x^2/5+C_2/x^2+2qC_4/x^3-C_4/x^4]m\\&\quad+[2\alpha_4x/5+C_4/x^4]m^3\\{}^{(1)}L(m)&=-\alpha_{-2}/m^2-\alpha_2m^2-\alpha_4m^4\end{aligned}$$

belonging to

$$\begin{aligned}{}^{(1)}r(x,m)&=-2C_4(m-1)m(m+1)(m+2)/x^5\\&\quad-2qC_4(3m(m+1)-1)/x^4\\&\quad-2(C_2m(m+1)+2q^2C_4)/x^3-2qC_2/x^2\\&\quad-\alpha_{-2}/qx+(\alpha_2/3-\alpha_4/15)m\\&\quad+(\alpha_2/3+2\alpha_4/15)m^2+2\alpha_4m^3/5\\&\quad+\alpha_4m^4/5-2qx(3\alpha_4m(m+1)\\&\qquad+5\alpha_2-\alpha_4)/15+2q^2\alpha_4x^2/5\end{aligned}$$

where C_i is the constant of integration in the equation with α_i on the right side.

Let us carry out the second-order calculations for the following special case (which is sufficiently general for the problem treated in the next section):

$$\begin{aligned}{}^{(1)}k(x,m)&=\alpha_2xm/3\\{}^{(1)}L(m)&=-\alpha_2m^2\end{aligned}$$

belonging to

$${}^{(1)}r(x,m)=-2q\alpha_2x/3+\alpha_2m(m+1)/3. \quad (13.1.3)$$

The coefficients of powers of m in the expansion of ${}^{(2)}k(x,m)$ satisfy equations similar to those satisfied by the coefficients in ${}^{(1)}k(x,m)$. Comparing (13.0.3) with (13.0.1) we see that the difference will be only that contributions from ${}^{(1)}k^2(x,m)$ will have to be added to some of the equations for ${}^{(1)}k_i(x)$ to obtain the equations for ${}^{(2)}k_i(x)$.

We require the expansion of ${}^{(2)}k(x,m)$ up to m^5; a particular solution can be found to be

$$\begin{aligned}{}^{(2)}k(x,m)&=[(\beta_2/3-\beta_4/15+\beta_6/21)x\\&\quad-(\beta_4/5-\beta_6/7)qx^2-(\alpha_2^2/45-4q^2\beta_6/35)x^3]m\\&\quad+[(2\beta_4/5-\beta_6/7)x-2q\beta_6x^2/7]m^3+3\beta_6xm^5/7\\{}^{(2)}L(m)&=-\beta_2m^2-\beta_4m^4-\beta_6m^6\end{aligned}$$

where β_i takes the place of α_i in the first approximation; β_{-2} and all the constants of integration have been put equal to zero so that our solution is not the most general one. Corresponding to this solution

$$\begin{aligned}{}^{(2)}r(x,m)&=(\beta_2/3-\beta_4/15+\beta_6/21)m\\&\quad+(\beta_2/3+2\beta_4/15-2\beta_6/21)m^2+(2\beta_4/5-\beta_6/7)m^3\\&\quad+(\beta_4/5+2\beta_6/7)m^4+3\beta_6m^5/7+\beta_6m^6/7\\&\quad-2qx(\beta_2/3+\delta-3\delta m+\beta_4m^2/5+2\beta_6m^3/7+\beta_6m^4/7)\\&\qquad-x^2(6q^2\delta+2\gamma m+2\gamma m^2)+2q\gamma x^3 \quad (13.1.4)\end{aligned}$$

where

$$\begin{aligned}\gamma&\equiv\alpha_2^2/45-4q^2\beta_6/35\\\delta&\equiv\beta_6/21-\beta_4/15.\end{aligned}$$

We are now free to choose in any manner (artificially or otherwise) the α_i,β_i in ${}^{(1)}r$ and ${}^{(2)}r$. Thus we are able to identify our perturbed potential function with a given potential function and from the corresponding perturbed k and L we can then write down the eigenvalues and normalized eigenfunctions for the given perturbation.

13.2 Stark effect

As an application of the formulas developed in the preceding section let us consider the differential equation

$$f''-(2q/x)f-(m(m+1)/x^2)f+2\epsilon xf+\lambda f=0 \quad (13.2.1)$$

where ϵ is a small parameter so that $2\epsilon xf$ is a small term compared to the others in the region where f is appreciably different from zero.

When $\epsilon=0$ the problem is type F so that the zero order eigenvalues are

$$\lambda={}^{(0)}L(n)=-q^2/n^2, \quad n-m+1=\text{integer}\geq 0.$$

The first-order terms in the perturbation are obtained by comparing (13.1.1) with $2x$. We see that we must take

$$\alpha_2=-3/q$$

and write

$$\lambda'=\lambda+\epsilon m(m+1)/q.$$

So that we artificially absorb the $\epsilon\alpha_2m(m+1)/3$ term in with λ. In this case the correction to the eigenvalues is obtained from the condition

$$\lambda'={}^{(0)}L(n)+\epsilon\,{}^{(1)}L(n).$$

To the first order, then,

$$\lambda=-q^2/n^2-\epsilon m(m+1)/q+\epsilon 3n^2/q$$

where $n-m+1$ is an integer ≥ 0.

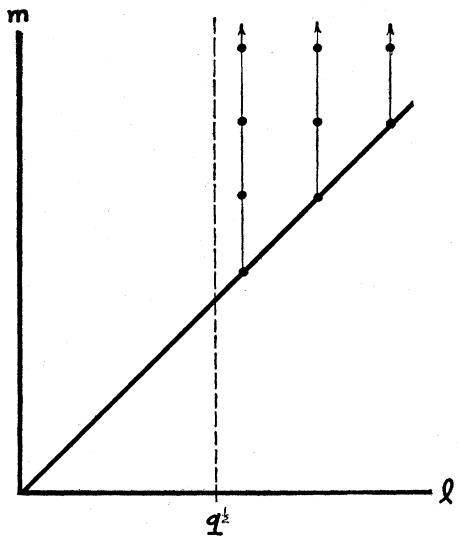


FIG. 6. Each dot represents a solution of (14.0.1) such that (14.0.4) exists.

For the eigenfunctions to this approximation we need

$$\begin{aligned} k(x,m) &= {}^{(0)}k(x,m)+\epsilon\,{}^{(1)}k(x,m) \\ &= m/x+q/m-\epsilon mx/q \\ L(m) &= {}^{(0)}L(m)+\epsilon\,{}^{(1)}L(m) \\ &= -q^2/m^2+3\epsilon m^2/q \end{aligned}$$

so that

$$\left.\begin{aligned} f_n{}^{n-1} &= 2^n(-q)^{n+1}n^{-n-\frac{1}{2}} \\ &\quad\times[-4q^3(2n)!+\epsilon n^3(2n+2)!]^{-\frac{1}{2}} \\ &\quad\times x^n\exp(qx/n)[-2q+\epsilon nx^2], \quad q<0 \\ f_n{}^{m-1} &= [\lambda-L(m)]^{-\frac{1}{2}}\left\{k(x,m)+\frac{d}{dx}\right\}f_n{}^m. \end{aligned}\right\} \quad (13.2.2)$$

To obtain the second-order terms in the perturbation we must compare ${}^{(2)}r(x,m)$ as given above (13.1.4) with zero. So that $\gamma=\delta=0$, we put

$$\beta_6=7/4q^4, \quad \beta_4=5/4q^4;$$

then

$${}^{(2)}r(x,m)=(m(m+1)-2qx)(\beta_2/3+m^2(m+1)^2/4q^4)$$

and, since this is to be zero, we must put

$$\beta_2=-3m^2(m+1)^2/4q^4$$

artificially—i.e. we must introduce this value of β_2 only *after* the ladder operations have been carried out.

To find the eigenvalues we can substitute this value of β_2 immediately. The constant term in ${}^{(2)}r(x,m)$ disappears so we can introduce the above λ' again and from

$$\lambda'={}^{(0)}L(n)+\epsilon\,{}^{(1)}L(n)+\epsilon^2\,{}^{(2)}L(n)$$

we obtain finally

$$\begin{aligned} \lambda=&-q^2/n^2+\epsilon(3n^2-m(m+1))/q \\ &-\epsilon^2(7n^6+5n^4-3n^2m^2(m+1)^2)/4q^4. \end{aligned} \quad (13.2.3)$$

The above values of α_2, β_6, β_4, and the artificial β_2 could also be used to find the eigenfunctions to the second order in ϵ.

The theory of the Stark effect leads to the following pair of equations (2, p. 403):

$$\left.\begin{aligned} &f_1''+((1+\beta)/x)f_1 \\ &\qquad -(m(m+1)/x^2)f_1+2\epsilon xf_1+\lambda f_1=0 \\ &f_2''+((1-\beta)/x)f_2 \\ &\qquad -(m(m+1)/x^2)f_2-2\epsilon xf_2+\lambda f_2=0 \end{aligned}\right\} \quad (13.2.4)$$

and the problem is to find the eigenvalues and eigenfunctions when λ, β are the same in each equation.

Comparing (13.2.4) with (13.2.1) and using (13.2.3) we can obtain the required eigenvalues. We first put $2q=-1-\beta$, $n=n_1$ in (13.2.3) and then put $2q=-1+\beta$, $n=n_2$ in (13.2.3); then, eliminating β between the two equations so obtained, we find

$$\begin{aligned} \lambda=&-1/(n_1+n_2)^2-3\epsilon(n_1{}^2-n_2{}^2) \\ &-\epsilon^2(n_1+n_2)^4(7n_1{}^2+7n_2{}^2+20n_1n_2-18m(m+1)+5)/4. \end{aligned}$$

The value of β is

$$\begin{aligned} \beta=&(n_1-n_2)/(n_1+n_2)-\epsilon(n_1+n_2)^2(3n_1n_2-m(m+1)) \\ &+\epsilon^2(n_1-n_2)(n_1+n_2)^5(n_1n_2-6m(m+1))/2n_1n_2. \end{aligned}$$

With q in terms of β the eigenfunctions can be obtained providing we keep in mind that q depends on β, and hence on m, only artificially. Eigenfunctions to the first order of approximation can be obtained from (13.2.2).

14. Interrelationship between Types

We have already mentioned several times the connection between type A and type E factorizations. Since types B, C, D are limiting forms of type A, and type F is a limiting form of type E, this connection means that all of our factorizations are interrelated. We now want to show explicitly the relationship between A and E.

For purposes of illustration it is sufficient to consider the special case

$$\frac{d^2Y}{dx^2}+\left[\frac{m(m+1)}{\cosh^2x}-2q\tanh x\right]Y+\lambda Y=0, \quad q>0 \quad (14.0.1)$$

of type E. The factorization is determined by

$$\begin{aligned} k(x,m) &= m\tanh x+q/m \\ L(m) &= -m^2-q^2/m^2. \end{aligned}$$

For $m^2\leq q$, $L(m)$ is an increasing function of m and so we look for Class I solutions. The key function would be

$$Y_l{}^l\sim\cosh^{l+1}x\exp(qx/(l+1)).$$

But this function does not satisfy the boundary conditions and so there are no solutions for $m^2\leq q$.

If $m^2>q$, $L(m)$ is a decreasing function of m and so we look for Class II solutions with the key function

$$Y_l{}^l \sim \cosh^{-l}x \exp(-qx/l)$$

belonging to the eigenvalue

$$\lambda=-l^2-q^2/l^2, \quad m-l=0, 1, 2, \cdots. \quad (14.0.2)$$

This key function does satisfy the boundary conditions when $l^2>q$ and can therefore be normalized. Moreover, successive applications of the m-raising operator will continue to produce functions which satisfy the boundary conditions. The eigenfunctions can therefore be represented by the dots in Fig. 6 where each ladder extends to infinity.

The same problem can be solved with a type A factorization. We introduce the value (14.0.2) for λ and look for a factorization which changes l, keeping m fixed. We use the formulas of Sec. 2.1 to introduce the new normal form

$$\frac{d^2F}{dz^2}-\left[\frac{l^2+q^2/l^2-\frac{1}{4}-2q\cos z}{\sin^2 z}\right]F+(m+\tfrac{1}{2})^2F=0$$

through the substitutions

$$x=\log\tan(z/2)$$
$$Y=\sin^{-\frac{1}{2}}z F.$$

If we now introduce the artificial parameter q' through $q=q'l$ our equation becomes

$$\frac{d^2F}{dz^2}-\left[\frac{(l-\frac{1}{2})(l+\frac{1}{2})+q'^2-2q'l\cos z}{\sin^2 z}\right]F$$
$$+(m+\tfrac{1}{2})^2F=0 \quad (14.0.3)$$

which is type A. Of course l now takes the place of m in the general discussion of Chapter 2. The factorization of (14.0.3) is given by

$$k(z, l)=(l-\tfrac{1}{2})\cot z-q'/\sin z$$
$$L(l)=(l-\tfrac{1}{2})^2.$$

$L(l)$ is an increasing function of l and so we can expect Class I solutions belonging to the eigenvalues

$$\lambda'=L(m+1)=(m+\tfrac{1}{2})^2.$$

(Here we allow m to play the role of l in the general discussion.) The key function is

$$F_m{}^m \sim \sin^{m+\frac{1}{2}-q'}(z/2)\cos^{m+\frac{1}{2}+q'}(z/2).$$

This function can be normalized on $0\leq z\leq\pi$ only if

$$m+\tfrac{1}{2}-q'>-\tfrac{1}{2}.$$

Moreover it is not difficult to see that if we try to use the operators to reach $F_m{}^l$ by taking $m-l$ steps down the ladder from $F_m{}^m$ we obtain a function which behaves like

$$\sin^{l+\frac{1}{2}-q'}(z/2)$$

near $z=0$. Therefore, if $F_m{}^l$ is to satisfy the boundary conditions, we must have

$$l+\tfrac{1}{2}-q'>-\tfrac{1}{2}$$

or

$$l>q'-1.$$

The eigenfunctions can therefore be represented by the dots in Fig. 7.

The restriction on l is less severe here than in Fig. 6. This is because the boundary condition for F is less severe than that for Y. In fact, we required that

$$\int_{-\infty}^{\infty} Y^2 dx \quad (14.0.4)$$

exist which, in terms of z, F, would mean that

$$\int_0^{\pi} (F^2/\sin^2 z)dz$$

must exist. This condition would obviously restrict F more than the one we actually used which was that

$$\int_0^{\pi} F^2 dz \quad (14.0.5)$$

must exist.

Thus we see that, except for the extra row of solutions in Fig. 7 due to the weaker boundary condition in this case, the two treatments we have given are simply the Class I and Class II factorizations of the same problem.

In the same way a relationship can be established between type B and F factorizations; as remarked at the end of Sec. 8.1, the Kepler problem was treated by Schrödinger as type B whereas we used the more natural type F approach. In quantum-mechanical applications the choice of factorization will depend on which approach leads to the physically proper normalization.

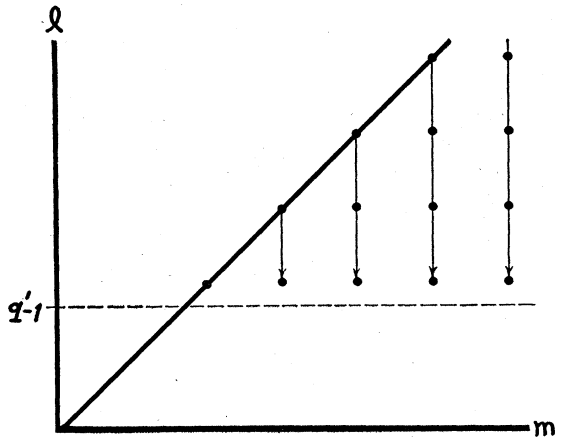


FIG. 7. Each dot represents a solution of (14.0.3) such than (14.0.5) exists. The bottom row of solutions has no counterpart it Fig. 6 because the boundary condition is weaker in this case.

In Sec. 4.2 we solved the spherical harmonics equation as a Class II problem; the factorization appeared there as type A rather than E only because the general type E factorization includes a special case (when $q=0$) which is also a special case of A.

Truesdell's technique which we will discuss immediately cannot be applied to type E or F factorizations; however it can be applied to the corresponding A or B factorizations.

15. Truesdell's F-Equation

Truesdell (49, p. 8) has considered the class of special functions which have the following properties in common: "(a) they satisfy ordinary linear differential equations of the second order; (b) they satisfy ordinary linear difference equations of the second order; (c) with suitable weight functions they form complete sets of orthogonal functions over a suitable interval; (d) they satisfy linear differential-difference relations."

As we have seen, the factorization method usually begins by replacing a second-order differential equation with a pair of first-order differential-difference relations —that is, it replaces property (a) with a pair of properties (d). Once this step is taken we have shown how the eigenvalues and normalized eigenfunctions can be written down immediately and how, in some cases, the corresponding matrix elements can be calculated. The fundamental characteristic of the factorization method is that it provides only those results which are of interest in the common physical problems— it does not provide *general* solutions of the original differential equation.

Truesdell is interested in the more general problem of providing "a general theory which motivates, discovers and coordinates the seemingly unconnected relations among the familiar special functions" (49, p. 7). These relations include the known expansions, nth derivative formulas, generating function representations, definite and contour integral representations and the integro-difference relations. He takes as a starting point the relation in (d) and his first step is to reduce this relation, through a change of both variables, to the form

$$\frac{\delta}{\delta z}F(z,\alpha)=F(z,\alpha+1)$$

which he calls the F-equation.

The condition that a recurrence relation provided by the factorization method can be reduced to the F-equation is only that $k(x,m)$ be linear in m. This means that Truesdell's techniques can be applied to the recurrence relations belonging to types A, B, C, D factorizations. But we have seen in the previous section that type E and F factorizations can be treated alternatively as A and B; therefore all the factorizations discussed in this report lead to F-equations and thus serve as starting points for the applications of Truesdell's results.

One special result in this connection has been thoroughly investigated by Duff (12). He has used the obvious formula

$$F(z,\alpha+n)=\delta^n/\delta z^n F(z,\alpha)$$

to obtain nth derivative expressions for all the normalized eigenfunctions considered in this report. The right side is, of course, determined by the key function.

16. Acknowledgments

We are pleased to acknowledge the helpful criticism of Professor A. F. C. Stevenson who has followed the factorization method through each phase of its development.

We are also very grateful to Mr. J. Kennedy for his help in the preparation of Chapter 6 and to Professor W. Opechowski for his valuable criticism of the same chapter.

Other staff members at the University of Toronto and the University of British Columbia have been unsparing in their willingness to help with various problems which arose during the preparation of this report.

17. Table of Factorizations

A detailed theoretical explanation of the use of the following table is given in Chapter 2 and Sec. 3.2. To solve a given second-order ordinary differential equation by the factorization method the steps to be taken are briefly as follows: 1. Transform the given equation to its normal form (2.1.1) by means of (2.1.2). 2. Identify the resulting $r(x,m)$ with one in the table. 3. Look up the reference in the last column. This reference is usually followed by the desired solutions; if not, the corresponding $k(x,m)$, $L(m)$ must be used to obtain the eigenvalues and normalized eigenfunctions as outlined in Sec. 2.7. It may be necessary to generalize step 2 by means of an artificial factorization as explained in Sec. 3.2.

In the table a, b, c, d, K, p, q, β, γ, and ν are constants. To conform with customary notations the variable x is sometimes replaced by r, y, z, θ, ρ, or ξ and the parameter m is sometimes replaced by l, M, n, or s.

Type	Name	$r(x,m)$	$k(x,m)$	$L(m)$	Reference to text
A	General type A	$-\dfrac{[a^2(m+c)(m+c+1)+d^2+2ad(m+c+\frac{1}{2})\cos a(x+p)]}{\sin^2 a(x+p)}$	$(m+c)a\cot a(x+p)+\dfrac{d}{\sin a(x+p)}$	$a^2(m+c)^2$	4.0.1
A	Associated spherical harmonics	$-\dfrac{m^2-\frac{1}{4}}{\sin^2\theta}$	$(m-\frac{1}{2})\cot\theta$	$(m-\frac{1}{2})^2$	4.1.3
A	Associated spherical harmonics	$\dfrac{l(l+1)}{\cosh^2 z}$	$l\tanh z$	$-l^2$	4.2.2

17. Table of Factorizations—*Continued*

Type	Name	$r(x, m)$	$k(x, m)$	$L(m)$	Reference to text
A	Generalized spherical harmonics	$-\frac{(m+\gamma)(m+\gamma-1)}{\sin^2\theta}$	$(m+\gamma-1)\cot\theta$	$(m+\gamma-1)^2$	4.3.1
A	Generalized spherical harmonics	$\frac{(l+\gamma-\frac{1}{2})(l+\gamma+\frac{1}{2})}{\cosh^2 z}$	$(l+\gamma-\frac{1}{2})\tanh z$	$-(l+\gamma-\frac{1}{2})^2$	4.3.2
A	Gegenbauer functions	$-\frac{m(m+1)}{\sin^2\theta}$	$m\cot\theta$	m^2	4.4.1
A	Symmetric top functions	$-\frac{(M-\frac{1}{2})(M+\frac{1}{2})+K^2-2MK\cos\theta}{\sin^2\theta}$	$(M-\frac{1}{2})\cot\theta-\frac{K}{\sin\theta}$	$(M-\frac{1}{2})^2$	4.5.1, see also 14.0.3
A	Harmonics with spin, magnetic pole	$-\frac{m(m+1)+\frac{1}{4}\pm(m+\frac{1}{2})\cos\theta}{\sin^2\theta}$	$m\cot\theta\pm\frac{1}{2\sin\theta}$	m^2	4.6.5, 4.7.1
A	Pöschl-Teller, hypergeometric	$-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sin^2\rho}$ $-\frac{(m+a+b-c-\frac{1}{2})(m+a+b-c+\frac{1}{2})}{\cos^2\rho}$	$(m+c-\frac{3}{2})\cot\rho$ $-(m+a+b-c-\frac{1}{2})\tan\rho$	$(2m+a+b-2)^2$	4.8.1, 4.9.3
A	Pöschl-Teller, hypergeometric	$-\frac{(m+a+b-c-\frac{1}{2})(m+a+b-c+\frac{1}{2})}{\sinh^2 y}$ $+\frac{(m+a-b-\frac{1}{2})(m+a-b+\frac{1}{2})}{\cosh^2 y}$	$(m+a+b-c-\frac{1}{2})\coth y$ $+(m+a-b-\frac{1}{2})\tanh y$	$-(2m+2a-c-1)^2$	4.8.2, 4.9.5
A	Hypergeometric	$-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sin^2\rho}$ $-\frac{(m+c-a-b-\frac{1}{2})(m+c-a-b+\frac{1}{2})}{\cos^2\rho}$	$(m+c-\frac{3}{2})\cot\rho$ $-(m+c-a-b-\frac{1}{2})\tan\rho$	$(2m+2c-a-b-2)^2$	4.9.4
A	Hypergeometric	$-\frac{(m+c-\frac{3}{2})(m+c-\frac{1}{2})}{\sinh^2 x}$ $+\frac{(m+a-b-\frac{1}{2})(m+a-b+\frac{1}{2})}{\cosh^2 x}$	$(m+c-\frac{3}{2})\coth x$ $+(m+a-b-\frac{1}{2})\tanh x$	$-(2m+a+c-b-2)^2$	4.9.6
B	General type B	$-d^2\exp(2ax)+2ad(m+c+\frac{1}{2})\exp(ax)$	$d\exp(ax)-m-c$	$-a^2(m+c)^2$	5.0.1
B	Confluent hypergeometric, Morse	$(-\frac{1}{4})\exp(2x)+(s+\frac{1}{2})\exp(x)$	$\exp(x)/2-s$	$-s^2$	5.1.3, 5.2.2
C	General type C	$-\frac{(m+c)(m+c+1)}{x^2}-\frac{b^2x^2}{4}+b(m-c)$	$\frac{m+c}{x}+\frac{bx}{2}$	$-2bm+b/2$	5.0.2
C	Confluent hypergeometric	$-\frac{(2m-\frac{1}{2})(2m+\frac{1}{2})}{y^2}-\frac{y^2}{16}$	artificial		5.1.8
C	System of identical oscillators	$-\frac{(n+s/2-\frac{1}{2})(n+s/2-\frac{3}{2})}{x^2}-x^2$	artificial (s is a constant here)		5.3.2
C	Bessel	$-\frac{m^2-\frac{1}{4}}{x^2}$	$\frac{m-\frac{1}{2}}{x}$	0 (see discussion)	5.4.1
D	General type D	$-(bx+d)^2+b(2m+1)$	$bx+d$	$-2bm$	6.0.1
D	Harmonic oscillator, meson fields	$-\xi^2$	modified treatment		6.1.1
D	Neutral meson field with sources	$-\xi^2-(\beta+\beta^*)\xi\pm(\beta-\beta^*)\frac{d}{d\xi}$	modified treatment		6.5.3, 6.5.5
D	Charged meson field with sources	$-\xi^2-(\beta\gamma+\beta^*\gamma^*)\xi\pm(\beta\gamma-\beta^*\gamma^*)\frac{d}{d\xi}$	modified treatment		6.7.2
E	General type E	$-\frac{m(m+1)a^2}{\sin^2 a(x+p)}-2aq\cot a(x+p)$	$ma\cot a(x+p)+\frac{q}{m}$	$a^2m^2-\frac{q^2}{m^2}$	7.0.1

17. Table of Factorizations—*Continued*

Type	Name	$r(x, m)$	$k(x, m)$	$L(m)$	Reference to text
E	Kepler problem in hypersphere	$-\frac{m(m+1)}{\sin^2 x}+2\nu\cot x$	$m\cot x-\frac{\nu}{m}$	$m^2-\frac{\nu^2}{m^2}$	7.1.2
E	Kepler problem in space of constant negative curvature	$-\frac{m(m+1)}{\sinh^2 x}+2\nu\coth x$	$m\coth x-\frac{\nu}{m}$	$-m^2-\frac{\nu^2}{m^2}$	7.2.2
E	Manning-Rosen	$-\frac{m(m+1)a^2}{\sinh^2 ar}+2a\nu\coth ar$	$ma\coth ar-\frac{\nu}{m}$	$-a^2m^2-\frac{\nu^2}{m^2}$	7.3.1
E	Rosen-Morse, Jacobi	$\frac{m(m+1)a^2}{\cosh^2 ax}-2aq\tanh ax$	$ma\tanh ax+\frac{q}{m}$	$-a^2m^2-\frac{q^2}{m^2}$	7.4.1, 7.5.2, see also 14.0.1
F	General type F	$-\frac{2q}{x}-\frac{m(m+1)}{x^2}$	$\frac{m}{x}+\frac{q}{m}$	$-\frac{q^2}{m^2}$	8.0.1
F	Kepler problem	$\frac{2}{r}-\frac{l(l+1)}{r^2}$	$\frac{l}{r}-\frac{1}{l}$	$-\frac{1}{l^2}$	8.1.3
F	Generalized Kepler problem	$\frac{2}{r}-\frac{(l+\gamma)(l+\gamma+1)}{r^2}$	$\frac{l+\gamma}{r}-\frac{1}{l+\gamma}$	$-\frac{1}{(l+\gamma)^2}$	8.3.1
F	Oscillating rotator	$\frac{2a}{r}-\frac{l(l+1)+a}{r^2}$	See discussion		8.6.1

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