

# 7

## The Eigenvalue Problem

One of the basic problems needing to be solved in quantum theory is the general eigenvalue problem, for some hermitian operator, say,  $A$ , with  $A^\dagger = A$ ,

$$A\psi_a(x) = \lambda_a\psi_a(x). \quad (1)$$

We shall learn how to solve such problems by purely algebraic techniques, without introducing wave functions and differential equations. For the moment, however, let us go back to the coordinate representation, and, in particular, let us choose  $A = H$ , where  $H$  is the Hamiltonian for a single particle in three dimensions, or for the two-particle problem after transformation to center of mass and relative coordinates. Keeping the center of mass fixed, the eigenvalue problem for the relative motion of the two-particle system is given by the Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi + V(x, y, z)\psi = E\psi. \quad (2)$$

If the potential is a function of the scalar distance  $r$  only, spherical coordinates will be natural and

$$-\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right)\psi + \frac{2\mu}{\hbar^2}(V(r) - E)\psi = 0. \quad (3)$$

Now, let

$$\psi(r, \theta, \phi) = R(r)Y(\theta, \phi) = R(r)\Theta(\theta)\Phi(\phi). \quad (4)$$

Substituting into the equation, and subsequently dividing by  $\psi = R\Theta\Phi$ , and then multiplying from the left with  $r^2$ , leads to a separation of the wave equation

$$\frac{r^2}{R} \left[ \frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \right] + \frac{2\mu r^2}{\hbar^2} (E - V(r)) = -\frac{1}{\Theta} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial \Theta}{\partial \theta} \right] - \frac{1}{\Phi \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2}. \quad (5)$$

Now, we have a function of  $r$  only, on the left-hand side of the equation, equaling a function of  $\theta$  and  $\phi$  only on the right. Hence, each function must be equal to the same constant, to be named,  $\lambda_0$ . By multiplying the right-hand side by  $\sin^2 \theta$ , we can further separate the  $\theta$  and  $\phi$ -dependent pieces. Letting the new separation constant be named  $m^2$ , we get the three separated equations

$$-\frac{\hbar^2}{2\mu} \left[ \frac{d^2 R}{dr^2} + \frac{2}{r} \frac{dR}{dr} \right] + \left[ \frac{\hbar^2}{2\mu r^2} \lambda_0 + V(r) \right] R(r) = ER(r), \quad (6)$$

$$-\frac{d^2 \Theta}{d\theta^2} - \cot \theta \frac{d\Theta}{d\theta} + \frac{m^2}{\sin^2 \theta} \Theta(\theta) = \lambda_0 \Theta(\theta), \quad (7)$$

$$-\frac{d^2 \Phi}{d\phi^2} = m^2 \Phi(\phi). \quad (8)$$

The solution to the last equation is trivial

$$\Phi(\phi) = e^{\pm im\phi}. \quad (9)$$

We shall prove later the separation constant,  $m$ , must be an integer. We shall defer the proof to later, but we note that it does *not* follow from the requirement that the wave function be single valued. It is  $\psi\psi^*$  and the probability density current,  $\vec{S}$ , that must be single valued, i.e., have the same value at  $\phi$  and  $(\phi + 2\pi)$ . The  $r$  and  $\theta$  equations can be simplified by eliminating the first derivative term to make them have the form of a 1-D Schrödinger equation. Because the volume element in spherical coordinates has the weighting factor  $r^2 \sin \theta$ , and we require the normalization

$$\int_0^\infty dr r^2 |R(r)|^2 \int_0^\pi d\theta \sin \theta |\Theta|^2 \int_0^{2\pi} d\phi |\Phi|^2 = 1, \quad (10)$$

(we will find it convenient to make each integral separately equal to unity), it will be useful to “one-dimensionalize” by transforming to new 1-D functions,  $u$ ,

$$rR(r) = u(r), \quad \sqrt{\sin \theta} \Theta(\theta) = u(\theta), \quad \Phi(\phi) = u(\phi). \quad (11)$$

The 1-D equations are then

$$\left( -\frac{d^2}{dr^2} + \frac{2\mu}{\hbar^2} \left[ V(r) + \frac{\hbar^2 \lambda_0}{2\mu r^2} \right] \right) u(r) = \frac{2\mu}{\hbar^2} E u(r) = \lambda u(r), \quad (12)$$

$$\left( -\frac{d^2}{d\theta^2} + \frac{(m^2 - \frac{1}{4})}{\sin^2 \theta} \right) u(\theta) = (\lambda_0 + \frac{1}{4}) u(\theta) = \lambda u(\theta), \quad (13)$$

$$-\frac{d^2 u}{d\phi^2} = m^2 u(\phi) = \lambda u(\phi). \quad (14)$$

The generic eigenvalue problem we want to solve has the form

$$\left(-\frac{d^2}{dx^2} + r(x, m)\right)u_{\lambda m}(x) = \lambda u_{\lambda m}(x). \quad (15)$$

The effective potential term often contains a parameter, named  $m$  in the generic equation, such as the parameter,  $m$ , in the  $\theta$  equation, or the parameter  $\lambda_0$  in the  $r$  equation.

One of the methods used by Schrödinger to solve this type of problem is the so-called factorization method, which naturally leads to a constructive process via ladder operators. The introduction of such ladder operators will ease the transition to the algebraic techniques, which we will use later to solve such eigenvalue problems, beginning with Chapter 14, where we reexamine many of these problems in a new light.

## A The Factorization Method: Ladder Operators

[A good reference for this method is: L. Infeld and T. E. Hull, *Reviews of Modern Physics* **23** (1951) 21. The table of factorizations at the end of the article gives a listing of 31 wave equations for which solutions are known in analytic form.]

In the factorization method, an attempt is made to solve the eigenvalue problem of eq. (15) by factoring the Schrödinger operator containing a second derivative operator into a product of two factors, each containing only a first derivative operator. Defining

$$\begin{aligned} O_+(m) &= -\frac{d}{dx} + k(x, m), \\ O_-(m) &= +\frac{d}{dx} + k(x, m), \end{aligned} \quad (16)$$

which through the basic second-order equation, eq. (15), satisfy the two equations

$$\begin{aligned} \text{I:} & \quad O_+(m)O_-(m)u_{\lambda m}(x) = [\lambda - \mathcal{L}(m)]u_{\lambda m}(x), \\ \text{II:} & \quad O_-(m+1)O_+(m+1)u_{\lambda m}(x) = [\lambda - \mathcal{L}(m+1)]u_{\lambda m}(x). \end{aligned} \quad (17)$$

For the specific case of the  $\theta$  equation, our eq. (13), the function

$$k(\theta, m) = \left(m - \frac{1}{2}\right) \cot \theta \quad (18)$$

will do the trick. Our equation (I) becomes

$$\begin{aligned} & \left(-\frac{d}{d\theta} + \left(m - \frac{1}{2}\right) \cot \theta\right) \left(+\frac{d}{d\theta} + \left(m - \frac{1}{2}\right) \cot \theta\right) u_{\lambda m}(\theta) \\ &= \left(-\frac{d^2}{d\theta^2} + \frac{(m^2 - \frac{1}{4})}{\sin^2 \theta} - \left(m - \frac{1}{2}\right)^2\right) u_{\lambda m}(\theta) \end{aligned}$$

$$= [\lambda - (m - \frac{1}{2})^2]u_{\lambda m}(\theta). \tag{19}$$

Equation (II) becomes

$$\begin{aligned} & \left( +\frac{d}{d\theta} + (m + \frac{1}{2}) \cot \theta \right) \left( -\frac{d}{d\theta} + (m + \frac{1}{2}) \cot \theta \right) u_{\lambda m}(\theta) \\ &= \left( -\frac{d^2}{d\theta^2} + \frac{(m^2 - \frac{1}{4})}{\sin^2 \theta} - (m + \frac{1}{2})^2 \right) u_{\lambda m}(\theta) \\ &= [\lambda - (m + \frac{1}{2})^2]u_{\lambda m}(\theta). \end{aligned} \tag{20}$$

The proposed factorization works for the  $\theta$  equation and leads in this case to

$$\mathcal{L}(m) = (m - \frac{1}{2})^2. \tag{21}$$

We will postpone the question, treated in detail by Infeld and Hull, for which “potentials” does the factorization work? Let us first prove a number of theorems.

**Theorem I:**

If  $u_{\lambda m}(x)$  is an eigenfunction of the generic equation with parameter,  $m$ , and eigenvalue  $\lambda$ , then  $[O_-(m)u_{\lambda m}(x)]$  is an eigenfunction of the equation with parameter,  $m - 1$ , and the same eigenvalue  $\lambda$ , and  $[O_+(m+1)u_{\lambda m}(x)]$  is an eigenfunction of the equation with parameter,  $m + 1$ , and the same eigenvalue  $\lambda$ .

That is,

$$\begin{aligned} O_-(m)u_{\lambda m}(x) &= \text{const.}u_{\lambda(m-1)}(x), \\ O_+(m+1)u_{\lambda m}(x) &= \text{const.}u_{\lambda(m+1)}(x). \end{aligned} \tag{22}$$

To see the first, act on equation (I) from the left with  $O_-(m)$  to give

$$O_-(m)O_+(m)\left[O_-(m)u_{\lambda m}\right] = [\lambda - \mathcal{L}(m)]\left[O_-(m)u_{\lambda m}\right]; \tag{23}$$

that is,  $O_-(m)u_{\lambda m}$  is a solution of equation (II), with  $m$  replaced by  $(m - 1)$ . Similarly, acting on equation (II) from the left with  $O_+(m + 1)$  gives

$$O_+(m+1)O_-(m+1)\left[O_+(m+1)u_{\lambda m}\right] = [\lambda - \mathcal{L}(m+1)]\left[O_+(m+1)u_{\lambda m}\right]; \tag{24}$$

that is,  $O_+(m + 1)u_{\lambda m}$  is a solution of equation (I), now with  $m$  replaced by  $m + 1$ . Thus,  $O_-(m)$  and  $O_+(m + 1)$  are  $m$  step-down, or step-up, operators that can ladder from a known solution to other solutions. Still to be answered: Are the new functions square-integrable if the original  $u_{\lambda m}$  were square-integrable? Do the  $m$ -ladders continue indefinitely to smaller or larger values? These questions still need to be answered. To see these, we need additional theorems.

**Theorem II:**

$$O_-(m) = O_+(m)^\dagger, \quad O_+(m) = O_-(m)^\dagger. \tag{25}$$

These relations follow from the adjoint properties of the two parts of the operators

$$\left[-\frac{d}{dx}\right] = \left[+\frac{d}{dx}\right]^\dagger; \quad k(x, m) = k(x, m)^\dagger. \tag{26}$$

We can use this theorem to investigate the square-integrability of  $u_{\lambda(m\pm 1)}$ . Assuming  $u_{\lambda m}$  is square-integrable, over an interval from  $a$  to  $b$ , consider

$$\begin{aligned}
 & \int_a^b dx u_{\lambda m+1}^*(x) u_{\lambda m+1}(x) \\
 &= |\text{const.}|^2 \int_a^b dx [O_+(m+1)u_{\lambda m}(x)]^* [O_+(m+1)u_{\lambda m}(x)] \\
 &= |\text{const.}|^2 \int_a^b dx u_{\lambda m}^*(x) O_-(m+1)O_+(m+1)u_{\lambda m}(x) \\
 &= |\text{const.}|^2 [\lambda - \mathcal{L}(m+1)] \int_a^b dx u_{\lambda m}^*(x) u_{\lambda m}(x). \tag{27}
 \end{aligned}$$

If the number  $[\lambda - \mathcal{L}(m+1)]$  is a positive number, the final result is a patently positive quantity, and  $u_{\lambda m+1}$  is square-integrable and can be normalized to one by an appropriate choice of the constant. If  $\mathcal{L}(m)$  is an increasing function of  $m$  (see Fig. 7.1), however, an  $m$ -value will come such that  $\mathcal{L}(m+1)$  will be greater than  $\lambda$ . Eq. (27) then would say that a patently positive quantity on the left-hand side of the equation would have to be a patently negative quantity on the right-hand side. This cannot be. Hence, the assumption that the solution  $u_{\lambda m}$  was square-integrable must have been wrong. The only way out of the soup comes if the  $m$  step-up process quits; i.e., if a maximum possible value of  $m$  exists,  $m_{\max}$ , such that

$$O_+(m_{\max} + 1)u_{\lambda m_{\max}}(x) = 0, \tag{28}$$

which would require

$$\lambda = \mathcal{L}(m_{\max} + 1). \tag{29}$$

Eq. (28) is a first-order equation, which can in principle always be integrated

$$-\frac{du_{\lambda m_{\max}}}{dx} + k(x, m_{\max} + 1)u_{\lambda m_{\max}} = 0. \tag{30}$$

For example, in the case of our  $\theta$  equation,

$$\frac{du_{\lambda m_{\max}}}{u_{\lambda m_{\max}}} = (m_{\max} + \frac{1}{2}) \cot \theta d\theta, \tag{31}$$

leading to

$$\ln u_{\lambda m_{\max}} = [\ln(\sin \theta)]^{m_{\max} + \frac{1}{2}}. \tag{32}$$

If we name

$$m_{\max} = l, \tag{33}$$

we can write this solution

$$u(\theta) = N_l \sin^{(l+\frac{1}{2})} \theta, \quad \Theta(\theta) = N_l \sin^l \theta; \tag{34}$$

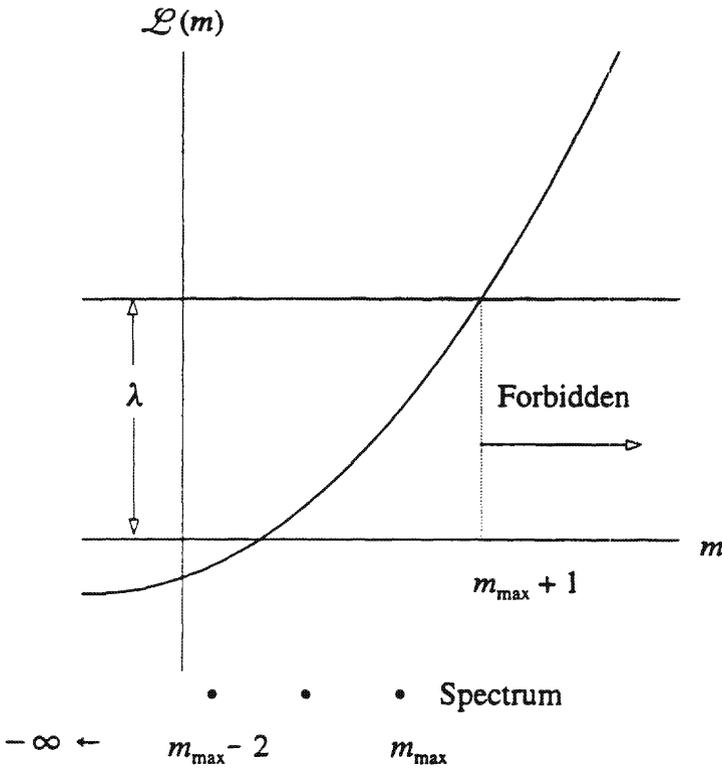


FIGURE 7.1. Case 1. A monotonically increasing  $\mathcal{L}(m)$ .

recalling that  $\sqrt{\sin \theta} \Theta(\theta) = u(\theta)$ . The normalization constant,  $N_l$ , can be evaluated to be

$$|N_l| = \sqrt{\frac{(2l+1)!!}{2(2l)!!}} = \sqrt{\frac{1 \cdot 3 \cdot 5 \cdots (2l+1)}{2[2 \cdot 4 \cdot 6 \cdots 2l]}}. \quad (35)$$

These considerations lead us to theorem IIIa.

Theorem IIIa:

If  $\mathcal{L}(m)$  is an increasing function of  $m$ , a highest value of  $m$  exists,  $m_{\max}$ , such that  $O_+(m_{\max} + 1)u_{\lambda, m_{\max}} = 0$ , and the eigenvalue,  $\lambda$ , is restricted by  $\lambda = \mathcal{L}(m_{\max} + 1)$ . In this case, normalized square-integrable eigenfunctions  $u_{\lambda, m}$  can be obtained from

$$u_{\lambda, m-1}(x) = O_-(m)u_{\lambda, m}(x), \quad (36)$$

where

$$O_-(m) \equiv \frac{O_-(m)}{\sqrt{[\lambda - \mathcal{L}(m)]}}. \quad (37)$$

That is, we can use a laddering process to ladder down from the eigenfunction with maximum possible  $m$  to arbitrary  $m$ , by repeated application of this operation.

Theorem IIIb:

If  $\mathcal{L}(m)$  is a decreasing function of  $m$ , (see, e.g., Fig. 7.2), a lowest value of  $m$  exists,  $m_{\min}$ , such that  $O_-(m_{\min})u_{\lambda m_{\min}} = 0$ , and the eigenvalue  $\lambda$  is restricted by  $\lambda = \mathcal{L}(m_{\min})$ . In this case, normalized, square-integrable eigenfunctions  $u_{\lambda m}$  can be obtained through a step-up procedure, starting with the eigenfunction with the minimum possible value of  $m$ , via

$$u_{\lambda m+1}(x) = \mathcal{O}_+(m+1)u_{\lambda m}(x), \quad (38)$$

where

$$\mathcal{O}_+(m+1) \equiv \frac{\mathcal{O}_+(m+1)}{\sqrt{[\lambda - \mathcal{L}(m+1)]}}. \quad (39)$$

Theorem IIIb follows from

$$\begin{aligned} & \int_a^b dx u_{\lambda m-1}^*(x) u_{\lambda m-1}(x) \\ &= |\text{const.}|^2 \int_a^b dx [O_-(m)u_{\lambda m}(x)]^* O_-(m)u_{\lambda m}(x) \\ &= |\text{const.}|^2 \int_a^b dx u_{\lambda m}^*(x) [O_+(m)O_-(m)u_{\lambda m}(x)] \\ &= |\text{const.}|^2 [\lambda - \mathcal{L}(m)] \int_a^b dx u_{\lambda m}^*(x) u_{\lambda m}(x). \end{aligned} \quad (40)$$

Now if  $[\lambda - \mathcal{L}(m)]$  is a positive quantity,  $u_{\lambda m-1}$  is square-integrable, if  $u_{\lambda m}$  is square-integrable. If  $\mathcal{L}(m)$  is a decreasing function of  $m$ , as in Fig. 7.2, however, a value of  $m$  would (in general) come such that  $[\lambda - \mathcal{L}(m-1)]$  would be a negative quantity, and again we would have a patently positive quantity on the left-hand side of the equation equal to a patently negative quantity on the right. The initial assumption that  $u_{\lambda m}$  be square-integrable must have been wrong. In the special case when  $\lambda = \mathcal{L}(m_{\min})$ , however, the laddering process quits at the value  $m_{\min}$ , and now no inconsistency exist.

In this case,

$$O_-(m_{\min})u_{\lambda m_{\min}} = 0, \quad (41)$$

$$+ \frac{du_{\lambda m_{\min}}}{dx} + k(x, m_{\min})u_{\lambda m_{\min}}(x) = 0. \quad (42)$$

In this case, if  $\mathcal{L}(m)$  is a *monotonic*, decreasing function of  $m$ , (see Fig. 7.2), the spectrum of allowed  $m$  values runs from  $m_{\min}$ ,  $m_{\min} + 1$ ,  $m_{\min} + 2$ ,  $\dots$ , on to  $+\infty$ ; the functions with higher  $m$  values being generated by repeated action with  $\mathcal{O}_+(m+1)$ .

So far, we have considered cases with  $\mathcal{L}(m)$  being monotonic increasing or decreasing functions of  $m$ . Our special example of the  $\theta$  equation, however, with  $\mathcal{L}(m) = (m - \frac{1}{2})^2$ , see Fig. 7.3, is an increasing function of  $m$  for positive  $m$  values and a decreasing function of  $m$  for negative  $m$  values. In this case, the laddering process will lead to square-integrable functions only if both a minimum value of

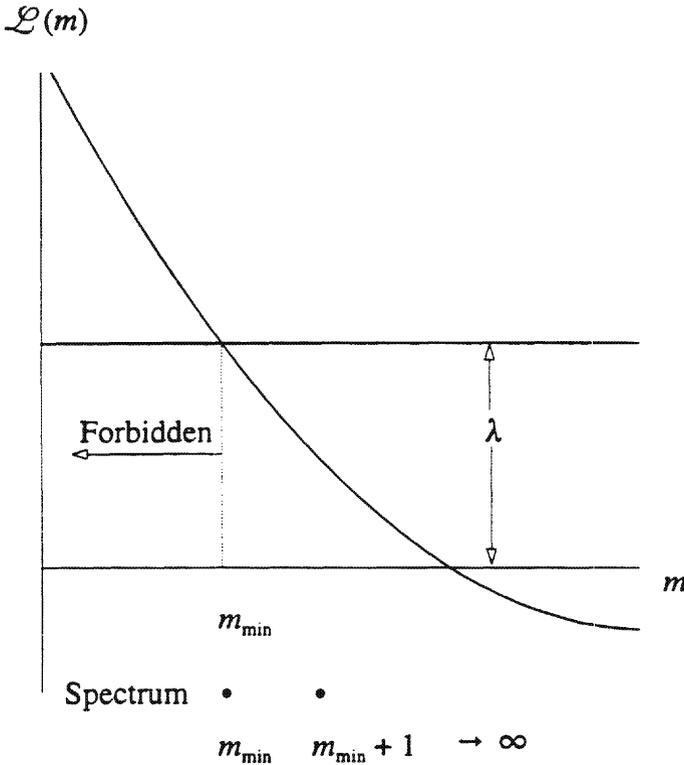


FIGURE 7.2. Case 2. A monotonically decreasing  $\mathcal{L}(m)$ .

$m$  and a maximum value of  $m$  exist. The spectrum of allowed  $m$  values is restricted to a finite number  $= (m_{\max} - m_{\min} + 1)$ .

In the special case of the  $\theta$ -equation, we have both

$$\lambda = \mathcal{L}(m_{\min}) = \mathcal{L}(m_{\max} + 1) = (m_{\min} - \frac{1}{2})^2 = (m_{\max} + \frac{1}{2})^2, \quad (43)$$

and thus 
$$m_{\min}^2 - m_{\min} = m_{\max}^2 + m_{\max}. \quad (44)$$

This quadratic equation for  $m_{\min}$  has the two roots,  $m_{\min} = -m_{\max}$  and  $m_{\min} = +(m_{\max} + 1)$ . Clearly, the last equation violates the meaning of  $m_{\min}$ . Thus, with  $m_{\max} \equiv l$ , the allowed  $m$  values range from  $+l$  in steps of one down to  $-l$ . Because  $(m_{\max} - m_{\min}) = 2l$  must be an integer, we have the result,  $2l$  must be an integer. Thus, seemingly  $l$  can be either an integer or a  $\frac{1}{2}$ -integer. Later, we shall prove only the integer values are allowed for the orbital or  $\theta$  equation.

Finally, the function  $\mathcal{L}(m)$  could be a decreasing function of  $m$  for large positive values of  $m$  and an increasing function of  $m$  for negative values of  $m$  (see Fig. 7.4). In this case for a  $\lambda < \mathcal{L}_{\max}$ , now two ranges of  $m$  values exist, one beginning at an  $m_{\min}$  and going in integer steps on to  $+\infty$ , and a second beginning at an  $m_{\max}$  and going in integer steps onto  $-\infty$ . If  $\lambda > \mathcal{L}_{\max}$ , then all  $m$  values would

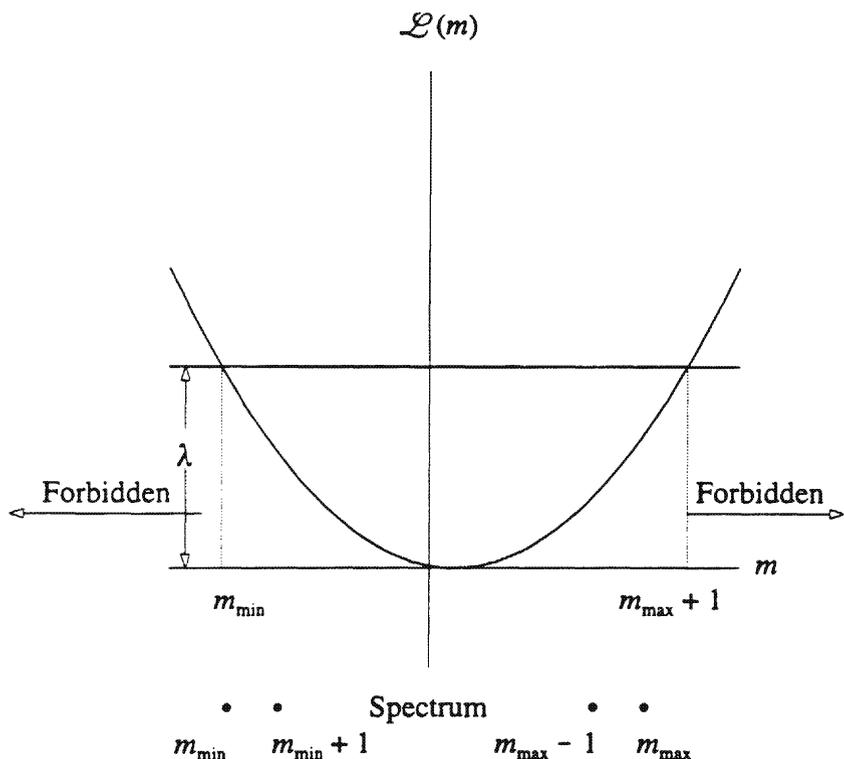


FIGURE 7.3. Case 3. An  $\mathcal{L}(m)$  with an allowed spectrum such that  $m_{\min} \leq m \leq m_{\max}$ .

be allowed. In this last case, therefore,  $\lambda$  also has a continuous spectrum for all values of  $\lambda > \mathcal{L}_{\max}$ . In this case, the normalization integral should have the delta function form

$$\int_{-\infty}^{\infty} dx u_{\lambda'm}^*(x) u_{\lambda m}(x) = \delta(\lambda' - \lambda). \tag{45}$$

With  $\lambda > \mathcal{L}(m)$  for all possible  $m$ , the normalized ladder operators,  $\mathcal{O}_+(m+1)$  and  $\mathcal{O}_-(m)$  exist. Moreover, they will preserve this normalization. If the  $u_{\lambda m}(x)$  are normalized according to eq. (45), then

$$\begin{aligned} \int_{-\infty}^{\infty} dx u_{\lambda'(m-1)}^*(x) u_{\lambda(m-1)}(x) &= \frac{\int_{-\infty}^{\infty} dx u_{\lambda'm}^* \left[ \mathcal{O}_+(m) \mathcal{O}_-(m) u_{\lambda m} \right]}{\sqrt{[\lambda' - \mathcal{L}(m)][\lambda - \mathcal{L}(m)]}} \\ &= \sqrt{\frac{[\lambda - \mathcal{L}(m)]}{[\lambda' - \mathcal{L}(m)]}} \int_{-\infty}^{\infty} dx u_{\lambda'm}^*(x) u_{\lambda m}(x) = \delta(\lambda' - \lambda). \end{aligned} \tag{46}$$

In this case, however, it may be difficult to find a solution for a starting value,  $u_{\lambda m_0}(x)$ .

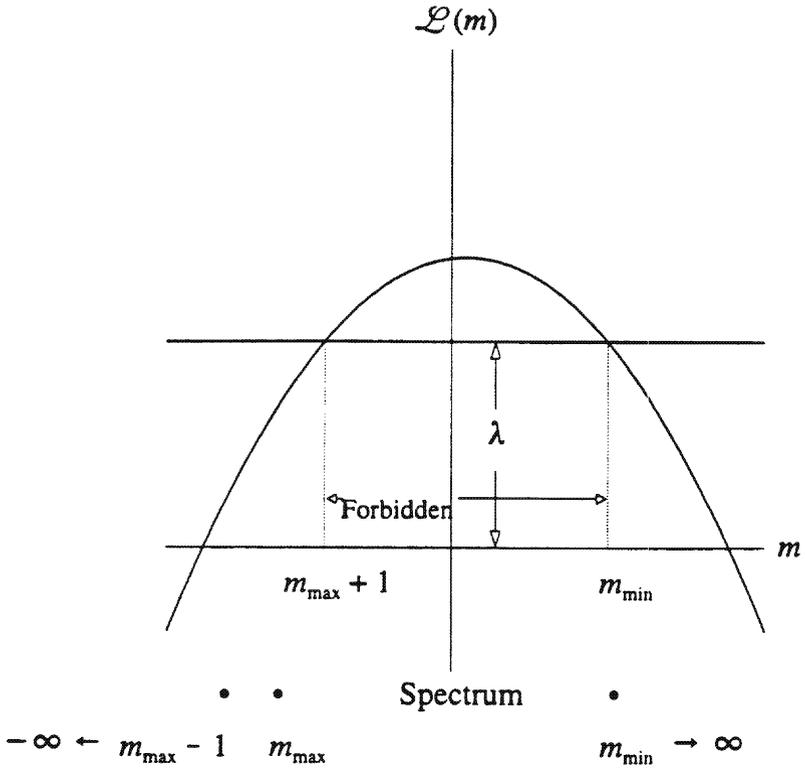


FIGURE 7.4. Case 4. An  $\mathcal{L}(m)$  with two allowed branches:  $m = m_{\max} \rightarrow -\infty$ , and  $m = m_{\min} \rightarrow +\infty$ .