



*The Abdus Salam*  
**International Centre for Theoretical Physics**



**SMR 1826 - 10**

**Preparatory School**  
to the  
**Winter College on Fibre Optics, Fibre Lasers and  
Sensors**

5 - 9 February 2007

**Second order differential operators and  
their eigenfunctions**

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# Second order differential operators and their eigenfunctions

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*Feb 23-27 2007*

## I. INTRODUCTION

A key concept in the study of waveguides is that of a mode. When traveling through a waveguide, a monochromatic light field can present one or several characteristic transverse profiles which remain invariant under propagation. These profiles are known as the *modes* of the waveguide, and they constitute a complete basis for representing any field propagating in it. A mode corresponds to what is known as an *eigenfunction* of the differential operator that describes the propagation of waves through the waveguide. Therefore, in order to understand it, it is a good idea to review the concept of eigenvalues and eigenfunctions for simple differential operators. In this lecture, we will discuss the simplest case, corresponding to only one variable. The behavior of multivariable operators is qualitatively similar. Since wave equations in linear optics are of second order, we will concentrate on the case of second order differential operators.

## II. HOMOGENEOUS SECOND ORDER LINEAR DIFFERENTIAL EQUATIONS AND THEIR SOLUTIONS

Consider a second order differential operator of the form:

$$\hat{D} = \frac{d^2}{dx^2} + p(x)\frac{d}{dx} + q(x), \quad (1)$$

where  $p(x)$  and  $q(x)$  are two functions of  $x$ . Notice that we could have written a more general operator where there is a function multiplying also the second derivative term. However, as we will see shortly, this is not necessary for the purposes of this section. (In subsequent sections, we will use operators that do have a function multiplying the second derivative, however.) The goal of this section is to revise the methods for solving homogeneous second order linear differential equations. These equations have the form:

$$\hat{D}f(x) = 0. \quad (2)$$

This equation is said to be homogeneous because the right-hand side is zero, i.e. there are no source/driving terms.

### A. Two independent solutions

Since this is a second order differential equation, there are two independent solutions. Consider, for example, the case where  $p$  and  $q$  are both constants, equal respectively to  $p_0$  and  $q_0$ . Then, it is easy to see that the solutions are exponentials of the form  $f(x) = \exp(ax)$ . The substitution of this form into the differential equation leads to

$$(a^2 + p_0a + q_0) \exp(ax) = 0. \quad (3)$$

There are two independent solutions, corresponding to the two different values of  $a$  for which  $a^2 + p_0a + q_0 = 0$ , that is

$$f_1(x) = \exp \left[ \left( \frac{p_0}{2} + \sqrt{\frac{p_0^2}{4} - q_0} \right) x \right], \quad f_2(x) = \exp \left[ \left( \frac{p_0}{2} - \sqrt{\frac{p_0^2}{4} - q_0} \right) x \right]. \quad (4)$$

Except for the case when  $q_0 = p_0^2/4$  (which will be discussed later), the full solution is then a linear combination of these solutions, i.e.

$$\begin{aligned} f(x) &= A_1 f_1(x) + A_2 f_2(x) \\ &= A_1 \exp \left[ \left( \frac{p_0}{2} + \sqrt{\frac{p_0^2}{4} - q_0} \right) x \right] + A_2 \exp \left[ \left( \frac{p_0}{2} - \sqrt{\frac{p_0^2}{4} - q_0} \right) x \right]. \end{aligned} \quad (5)$$

When solving a real problem where initial or boundary conditions must be met, these conditions set the values of the constants  $A_1$  and  $A_2$ . When  $p(x)$  and  $q(x)$  are not constant, the solutions can be more complicated, but there are always two independent solutions that are not simply multiples of each other.

### B. Wronskian

While the two solutions are always globally linearly independent, they can be locally multiples of each other in the sense that the ratio of their derivative and their value are equal:

$$\frac{f_1'(x)}{f_1(x)} = \frac{f_2'(x)}{f_2(x)}. \quad (6)$$

That is, for a given  $x$ , if the two functions are scaled to have the same magnitude, there is a chance that they might also have the same slope. This would represent a problem,

for example, if a point  $x_0$  where this were true happened to be the point at which initial conditions for the differential equation are prescribed:

$$f(x_0) = A_1 f_1(x_0) + A_2 f_2(x_0), \quad (7)$$

$$f'(x_0) = A_1 f_1'(x_0) + A_2 f_2'(x_0). \quad (8)$$

The solution for the constants is

$$A_1 = \frac{f(x_0)f_2'(x_0) - f'(x_0)f_2(x_0)}{f_1(x_0)f_2'(x_0) - f_1'(x_0)f_2(x_0)}, \quad (9)$$

$$A_2 = \frac{f'(x_0)f_1(x_0) - f(x_0)f_1'(x_0)}{f_1(x_0)f_2'(x_0) - f_1'(x_0)f_2(x_0)}. \quad (10)$$

But the denominator of these expressions vanishes if the above condition, Eq. (6), is true at  $x_0$ . The Wronskian is defined precisely as the combination in the denominator in Eqs. (9,10):

$$w(x) = f_1(x)f_2'(x) - f_1'(x)f_2(x). \quad (11)$$

The two solutions are locally linearly independent when the Wronskian is different from zero.

Notice that, up to a global constant, the Wronskian can be found even if the two solutions  $f_1$  and  $f_2$  are not known. Consider the derivative of the Wronskian:

$$w'(x) = [f_1(x)f_2'(x) - f_1'(x)f_2(x)]' = f_1(x)f_2''(x) - f_1''(x)f_2(x). \quad (12)$$

Now substitute, from the original differential equation,  $f_n''(x) = -p(x)f_n'(x) - q(x)f_n(x)$ :

$$\begin{aligned} w'(x) &= f_1(x)[-p(x)f_2'(x) - q(x)f_2(x)] - [-p(x)f_1'(x) - q(x)f_1(x)]f_2(x) \\ &= -p(x)[f_1(x)f_2'(x) - f_1'(x)f_2(x)] \\ &= -p(x)w(x), \end{aligned} \quad (13)$$

or

$$\frac{w'(x)}{w(x)} = -p(x). \quad (14)$$

The indefinite integral of both sides gives

$$\ln[w(x)] = -P(x) + c_0, \quad (15)$$

or

$$w(x) = w_0 \exp[-P(x)], \quad (16)$$

where  $c_0$  and  $w_0$  are constants, and

$$P(x) = \int_{x_0}^x p(x') dx'. \quad (17)$$

It is surprising that the functional form of the Wronskian is independent of  $q(x)$ .

### C. Finding the second solution from the first

Now, how do we find the two independent solutions? This is not so trivial. It turns out, however, that if somehow we know one of the solutions (either by inspection or by applying some technique), we can calculate the second. To see this, assume that we know  $f_1(x)$ . Then, write the second solution as a product of two unknown functions:

$$f_2(x) = M(x)u(x). \quad (18)$$

The substitution of this product into the differential equation gives

$$\begin{aligned} 0 &= \hat{D}f_2(x) = \hat{D}[M(x)u(x)] \\ &= [M(x)u(x)]'' + p(x)[M(x)u(x)]' + q(x)[M(x)u(x)] \\ &= M(x)u''(x) + [2M'(x) + p(x)M(x)]u'(x) + [M''(x) + p(x)M'(x) + q(x)M(x)]u(x) \\ &= M(x)u''(x) + [2M'(x) + p(x)M(x)]u'(x) + [\hat{D}M(x)]u(x). \end{aligned} \quad (19)$$

Notice that the last term vanishes if we choose  $M(x) = f_1(x)$  because  $\hat{D}f_1(x) = 0$ , so Eq. (19) becomes a first order equation in  $u'(x)$ :

$$f_1(x)u''(x) + [2f_1'(x) + p(x)f_1(x)]u'(x) = 0, \quad (20)$$

which after some rearranging becomes

$$\frac{u''(x)}{u'(x)} = -2\frac{f_1'(x)}{f_1(x)} - p(x). \quad (21)$$

The indefinite integral of both sides gives

$$\ln[u'(x)] = -2\ln[f_1(x)] - P(x) + c_0. \quad (22)$$

The exponential of both sides gives then

$$u'(x) = \frac{w_0}{f_1^2(x)} \exp[-P(x)] = \frac{w(x)}{f_1^2(x)}, \quad (23)$$

where we used Eq. (16) in the last step. Finally, this expression can also be integrated to give

$$u(x) = \int_{x_0}^x \frac{w(x')}{f_1^2(x')} dx' + c_1, \quad (24)$$

so the second solution is given by

$$f_2(x) = f_1(x)u(x) = f_1(x) \int_{x_0}^x \frac{w(x')}{f_1^2(x')} dx'. \quad (25)$$

Notice that, without loss of generality, the second integration constant  $c_1$  was set to zero, because if it were different from zero it would only add some amount of the first solution, and this can be accounted for in the final linear combination.

To test this solution, consider the example mentioned earlier where  $p(x) = p_0$  and  $q(x) = q_0$ , and insert the form of the first solution given in Eq. (4) into Eq. (25) to see if you can recover the second solution. This should be possible provided  $q_0 \neq p_0^2/4$ . If  $q_0 = p_0^2/4$ , the prescription in Eq. (25) gives the independent second solution that cannot be found simply by inspection. Can you find it?

#### D. Finding the first solution: the Frobenius method

Now, the hard part is finding the first solution. Except in simple cases like the example given earlier, one cannot find the first solution analytically. Therefore, it is necessary to find it as a series expansion. The method for doing this is known as the method of Frobenius. When expanding a function as a series, one of course has first to pick a point  $x_0$  around which the expansion is performed. Once this point is chosen, the series takes the form

$$f_1(x) = (x - x_0)^\gamma \sum_{n=0}^{\infty} a_n (x - x_0)^n. \quad (26)$$

Notice that this is not a strict Taylor series, due to the power of  $\gamma$  in front. This is to allow for the possibility that the function might diverge at  $x = x_0$  as some negative power, or grow as a fractional positive power (e.g. as a square root). Because  $f_1$  is going to have a global constant  $A_1$  in front, we can set, without loss of generality,  $a_0 = 1$ .

Let's talk now about how to choose  $x_0$ . There are many cases of practical interest (especially in the equations that describe the transverse modes of waveguides) where the functions  $p$  and  $q$  diverge at some value of  $x$ . It turns out that the Frobenius method still works in this case, as long as  $p$  has at most a simple pole and  $q$  a second order pole. In fact,

the regions of convergence of the series is maximized if we choose  $x_0$  to coincide with these singularities, if they exist. To see this, let us multiply the differential equation by  $(x - x_0)^2$  and write it in the following form:

$$(x - x_0)^2 f_1''(x) + [(x - x_0)p(x)] (x - x_0) f_1'(x) + [(x - x_0)^2 q(x)] f_1(x) = 0. \quad (27)$$

The substitution of Eq. (26) into this equation gives

$$\begin{aligned} & (x - x_0)^\gamma \sum_{n=0}^{\infty} (\gamma + n)(\gamma + n - 1) a_n (x - x_0)^n \\ & + [(x - x_0)p(x)] (x - x_0)^\gamma \sum_{n=0}^{\infty} (\gamma + n) a_n (x - x_0)^n \\ & + [(x - x_0)^2 q(x)] (x - x_0)^\gamma \sum_{n=0}^{\infty} a_n (x - x_0)^n = 0. \end{aligned} \quad (28)$$

Notice first that the factor of  $(x - x_0)^\gamma$  can be factored and eliminated. Secondly, the factors in this equations are the functions  $[(x - x_0)p(x)]$  and  $[(x - x_0)^2 q(x)]$ , which are analytic at  $x = x_0$  if  $p$  has at most a single pole and  $q$  has a second order pole. These combinations can then be expanded in Taylor series as

$$[(x - x_0)p(x)] = \sum_{m=0}^{\infty} P_m (x - x_0)^m, \quad (29)$$

$$[(x - x_0)^2 q(x)] = \sum_{m=0}^{\infty} Q_m (x - x_0)^m. \quad (30)$$

From this, one can rearrange the series into one big series expression that equals zero for all values of  $x$ . This means that the coefficient of each power of  $(x - x_0)^n$  must vanish independently. From here, one finds an infinite set of equations, the first of which (known as indicial) determines the exponent  $\gamma$ , and the subsequent ones serve to find the coefficients  $a_n$ . Instead of solving the general case, let us consider an example that is important in waveguide theory.

The Bessel equation has the form:

$$x^2 f''(x) + x f'(x) + (x^2 - \nu^2) f(x) = 0. \quad (31)$$

That is, the second order operator has the following form:

$$\hat{D} = \frac{d^2}{dx^2} + \frac{1}{x} \frac{d}{dx} + \left(1 - \frac{\nu^2}{x^2}\right). \quad (32)$$



It is easy to see that the natural choice for  $x_0$  in this case is zero, where  $p = 1/x$  and  $q = 1 - \nu^2/x^2$  are singular. Further, in this case there is no need to expand  $[(x - x_0)p(x)]$  and  $[(x - x_0)^2q(x)]$  in Taylor series, as they are already explicitly in the form of (very short!) series, namely 1 and  $-\nu^2 + x^2$ , respectively. The substitution of the series form in Eq. (26) with  $x_0 = 0$  into Eq. (31) then gives

$$x^\gamma \sum_{n=0}^{\infty} (\gamma + n)(\gamma + n - 1)a_n x^n + x^\gamma \sum_{n=0}^{\infty} (\gamma + n)a_n x^n + (x^2 - \nu^2)x^\gamma \sum_{n=0}^{\infty} a_n x^n = 0, \quad (33)$$

which, after dividing by  $x^\gamma$  and reordering, can be written as

$$\sum_{n=0}^{\infty} [(\gamma + n)^2 - \nu^2]a_n x^n + \sum_{n=0}^{\infty} a_n x^{n+2} = 0. \quad (34)$$

In order to combine these two sums, we must first change the indices, such that the powers of  $x$  are the same. This is done by letting  $m = n$  in the first sum and  $m = n + 2$  in the second. Of course, now the second sum will start at  $m = 2$  so the terms corresponding to  $n = 0, 1$  in the first sum must be written separately. The result is:

$$(\gamma^2 - \nu^2) + [(\gamma + 1)^2 - \nu^2]a_1 x + \sum_{m=2}^{\infty} \{[(\gamma + m)^2 - \nu^2]a_m + a_{m-2}\}x^m = 0. \quad (35)$$

Here, we used the fact that  $a_0 = 1$ . Because this equation holds for all  $x$ , then the constant coefficient of each power of  $x$  must vanish independently. Consider first the constant term. Setting this term to zero gives what is known as the indicial equation, which in this case becomes

$$\gamma^2 - \nu^2 = 0 \rightarrow \gamma = \pm\nu. \quad (36)$$

These two choices of the sign correspond to the two solutions. However, as we will see later, the negative choice does not lead to the second solution when  $\nu$  is an integer or a half integer (which is the case in waveguide problems). Let us then concentrate on the first solution only, corresponding to  $\gamma = \nu$  (assuming  $\nu \geq 0$ ).

The coefficient of the linear term must also be set to zero, that is,

$$[(\gamma + 1)^2 - \nu^2]a_1 = (2\nu + 1)a_1 = 0, \quad (37)$$

where we used  $\gamma = \nu$  in the second step. Notice that the only way for satisfying this equation is to make  $a_1 = 0$ . Finally, the rest of the equations, corresponding to the coefficients of all higher powers of  $x$  vanishing independently, can be solved generically as

$$[(\gamma + m)^2 - \nu^2]a_m + a_{m-2} = (2m\nu + m^2)a_m + a_{m-2} = 0. \quad (38)$$

This leads to the recursion relation

$$a_n = -\frac{a_{n-2}}{n(n+2\nu)}. \quad (39)$$

Let's make a remark about this result. Notice that if we chose the minus sign in Eq. (36), the plus sign in the denominator would be a minus sign. For this reason, this recursion relation would fail if  $\nu$  were an integer or half integer, because there would be a value of  $n$  that would make the expression diverge. In this case, the second solution must be sought with the procedure explained earlier. This second solution corresponds to a Bessel function of the second kind, which diverges at  $x = 0$ . In simple, typical waveguide problems, this solution is often discarded because of this divergence, so we concentrate on the first solution. For the positive choice of the sign, there is no problem. This first solution is precisely what is known as the Bessel function of the first kind,  $J_\nu(x)$ . In Fig. 1 we show how the series solution we found approaches the function inbuilt in the computational software program *Mathematica*. For illustration purposes, we show the series truncated at several maximum values of  $m$ , to see how the region of validity increases.

### III. SELF-ADJOINT OPERATORS

Many of you are probably familiar with the concept of a self-adjoint (or Hermitian) matrix. A matrix  $\mathbb{M}$  of this type satisfies the following property

$$\mathbf{v}^* \cdot (\mathbb{M}\mathbf{u}) = (\mathbb{M}\mathbf{v})^* \cdot \mathbf{u}, \quad (40)$$

where  $\mathbf{u}$  and  $\mathbf{v}$  are two arbitrary vectors. In order to extend the concept of self-adjointness to second order differential operators, it is important to first extend the concept of “dot” or inner product to continuous functions instead of discrete vectors. The inner product of two complex functions  $u(x)$  and  $v(x)$  is defined as

$$\langle v, u \rangle = \int_{x_0}^{x_1} v^*(x)u(x)dx, \quad (41)$$

where  $x_0$  and  $x_1$  define the limits of the region of interest, and the complex conjugate in the first function is inserted so that, for any complex function, the inner product with itself gives a non-negative real number.

### A. Canonical form of a self-adjoint operator

Consider a general second order differential operator

$$\hat{\mathcal{D}} = p_0(x) \frac{d^2}{dx^2} + p_1(x) \frac{d}{dx} + p_2(x). \quad (42)$$

Notice that, because we are not explicitly considering a differential equation, we include a function multiplying the second derivative for the sake of generality. In analogy with Eq. (40), this differential operator is self-adjoint if

$$\langle v, \hat{\mathcal{D}}u \rangle = \langle \hat{\mathcal{D}}v, u \rangle + [] \Big|_{x_0}^{x_1}, \quad (43)$$

where the last term represents terms evaluated at the endpoints. Substituting the explicit form of the operator into the left-hand side of this equation, we get

$$\langle v, \hat{\mathcal{D}}u \rangle = \int_{x_0}^{x_1} v^* (p_0 u'' + p_1 u' + p_2 u) dx. \quad (44)$$

We can now remove all the derivatives from  $u$  by using integration by parts:

$$\begin{aligned} \langle v, \hat{\mathcal{D}}u \rangle &= \int_{x_0}^{x_1} v^* (p_0 u'' + p_1 u' + p_2 u) dx \\ &= (v^* p_0 u' + v^* p_1 u) \Big|_{x_0}^{x_1} + \int_{x_0}^{x_1} [-(v^* p_0)' u' - (v^* p_1)' u + v^* p_2 u] dx \\ &= [v^* p_0 u' + v^* p_1 u - (v^* p_0)' u] \Big|_{x_0}^{x_1} + \int_{x_0}^{x_1} [(v^* p_0)'' u - (v^* p_1)' u + v^* p_2 u] dx \\ &= [p_0 (v^* u' - v'^* u) + (p_1 - p_1') v^* u] \Big|_{x_0}^{x_1} \\ &\quad + \int_{x_0}^{x_1} [p_0^* v'' + (2p_0' - p_1)^* v' + (p_0'' - p_1' + p_2)^* v]^* u dx \\ &= [p_0 (v^* u' - v'^* u) + (p_1 - p_1') v^* u] \Big|_{x_0}^{x_1} + \langle \hat{\mathcal{D}}v, u \rangle, \end{aligned} \quad (45)$$

where

$$\hat{\mathcal{D}} = p_0^*(x) \frac{d^2}{dx^2} + [2p_0'(x) - p_1(x)]^* \frac{d}{dx} + [p_0''(x) - p_1'(x) + p_2(x)]. \quad (46)$$

The operator  $\hat{\mathcal{D}}$  is then self-adjoint if it equals  $\hat{\mathcal{D}}$ , i.e. if

$$p_0 = p_0^*, \quad (47)$$

$$p_1 = 2p_0'^* - p_1^*, \quad (48)$$

$$p_2 = p_0''^* - p_1'^* + p_2^*. \quad (49)$$

The condition in Eq. (47) states that  $p_0$  is real. The condition in Eq. (48) can then be written out as

$$\Re(p_1) = p'_0, \quad (50)$$

where  $\Re$  denotes the real part. Finally, the real and imaginary parts of condition in Eq. (48) become then

$$\Re(p'_1) = p''_0, \quad (51)$$

$$2\Im(p_2) = -\Im(p'_i), \quad (52)$$

where  $\Im$  denotes the imaginary part. In other words, the operator is self adjoint if the coefficients are of the following general form:

$$p_0(x) = \alpha(x), \quad (53)$$

$$p_1(x) = \alpha'(x) + 2i\gamma(x), \quad (54)$$

$$p_2(x) = \beta(x) + i\gamma'(x). \quad (55)$$

For real operators,  $\gamma = 0$ , so the operator acting on a function takes the simple canonical form

$$\hat{D}u(x) = [\alpha(x)u'(x)]' + \beta(x)u(x). \quad (56)$$

## B. Making a regular operator self-adjoint

What if we are dealing with an operator which does not have the canonical form in Eq. (56), specifically if it is instead of the form in Eq. (1)? We show now that this operator can be easily transformed into the canonical form by writing the function the operator acts on,  $f$ , as a product of two functions,  $M$  and  $u$ , and applying the product rule:

$$\hat{D}f(x) = \hat{D}[M(x)u(x)] = Mu'' + (2M' + pM)u' + (M'' + pM' + qM)u. \quad (57)$$

Therefore,  $\hat{D}f = \hat{D}u$  if

$$\alpha = M, \quad (58)$$

$$\alpha' = 2M' + pM, \quad (59)$$

$$\beta = M'' + pM' + qM \quad (60)$$

The combination of Eqs. (58) and (59) gives  $M' + pM = 0$ , so  $\alpha = M$  is the Wronskian  $w$ . It is easy to see from Eq. (60) that  $\beta = w'' + pw' + qw = (-pw)' + p(-pw) + qw = (q - p')w$ . Therefore,

$$\hat{D}f = (wu')' + (q - p')wu. \quad (61)$$

As an exercise, transform the differential operator of the Bessel equation in Eq. (31) into self-adjoint form.

#### IV. MODES

It was discussed earlier that, if the Wronskian vanishes at some value of the variable, it is impossible to find a (unique) solution that satisfies initial conditions at that value. Let us now discuss the case of boundary conditions, where the value of the function, its derivative, or some combination, is specified at two different values of the variable that constitute the ends of the region of interest. Consider, for example, the case of Dirichlet boundary conditions, where the values of  $f$  at the points  $x_a$  and  $x_b$  are prescribed. As in the case of initial conditions, there are situations in which a (unique) solution that matches the prescribed boundary conditions does not exist. However, it turns out that, since these conditions are not both at the same location, there is no simple function like the Wronskian that can alert us of this problem. There is, nevertheless, a condition which, if satisfied, guarantees the existence of a solution. In this section we will derive this condition.

Consider the case when we want to find a solution to the differential equation (2) for  $x \in [x_0, x_1]$ , and given the boundary conditions  $f(x_a), f(x_b)$ . As we know, there are two independent solutions to this equation, namely  $f_1(x)$  and  $f_2(x)$ . An easy way to find a solution to the boundary value problem is to define two new, mutually linearly independent functions,  $f_a(x)$  and  $f_b(x)$ , given by the following combinations of  $f_1$  and  $f_2$ :

$$f_a(x) = f_2(x_a)f_1(x) - f_1(x_a)f_2(x), \quad (62)$$

$$f_b(x) = f_2(x_b)f_1(x) - f_1(x_b)f_2(x), \quad (63)$$

$$(64)$$

It is easy to see that  $f_a(x_a) = f_b(x_b) = 0$ . Therefore, provided that  $f_a(x_b) \neq 0$  and  $f_b(x_a) \neq 0$ ,

the solution to the boundary value problem is simply

$$f(x) = \frac{f(x_a)}{f_b(x_a)}f_b(x) + \frac{f(x_b)}{f_a(x_b)}f_a(x). \quad (65)$$

However, if  $f_a(x_b)$  or  $f_b(x_a)$  vanish, the boundary value problem is not well defined. Notice that, if this is the case, at least one of these functions vanish at both boundaries without being identically zero in between. Such a solution that happens to vanish at the endpoints is called a “mode”. When solving differential equations with nonzero boundary conditions, modes represent a problem. As we will see in the next section, there are other types of physical problems in which modes are actually a good thing. Before this, however, let us find a condition that can predict whether modes are possible or not.

### A. Conditions for modes

Let us, without loss of generality, write the differential equation in self-adjoint form  $\hat{\mathcal{D}}u(x) = 0$ , as explained earlier. This means that, instead of dealing with the function  $f(x)$ , we will use  $u(x)$ . For a mode,  $u(x_a) = u(x_b) = 0$ . To find the condition, consider the inner product of  $u(x)$  and  $\hat{\mathcal{D}}u(x)$ :

$$0 = \langle u, \hat{\mathcal{D}}u \rangle = \int_{x_a}^{x_b} u^* [(\alpha u')' + \beta u] dx. \quad (66)$$

By integrating by parts the first term and remembering that  $u$  vanishes at the endpoints, we find the condition

$$0 = \int_{x_a}^{x_b} [\beta(x)|u(x)|^2 - \alpha(x)|u'(x)|^2] dx. \quad (67)$$

It is easy to see that, if  $\alpha$  and  $\beta$  have opposite signs over all  $x \in [x_a, x_b]$ , the only way in which Eq. (67) can be satisfied is if  $u(x)$  is identically zero everywhere in this interval. This means that modes cannot exist if the following condition is satisfied:

$$\alpha(x)\beta(x) < 0, \quad x \in [x_a, x_b]. \quad (68)$$

It must be noted that the fact that this condition is not satisfied does not imply that there will be modes, only that there is a possibility of having modes. To see this consider the two following examples: First, consider the operator

$$\hat{\mathcal{D}} = \frac{d^2}{dx^2} - k^2. \quad (69)$$

It is easy to see that  $\alpha\beta = -k^2 < 0$  so there are no modes. This is true, because the solutions are proportional to  $\exp(\pm kx)$ , and no combination of these exponentials can be made to vanish at two points without vanishing everywhere else. On the other hand, if we have the operator

$$\hat{D} = \frac{d^2}{dx^2} + k^2, \quad (70)$$

then  $\alpha\beta = k^2 > 0$ , so there might be modes, which makes sense because the two independent solutions are now  $\sin(kx)$  and  $\cos(kx)$ , so there are modes if  $x_a$  and  $x_b$  are separated by an integer multiple of  $2\pi/k$ .

## V. STÜRM-LIOUVILLE PROBLEMS

A Stürm-Liouville problem is the continuous analogue of a matrix eigenvalue equation. Consider the following differential equation

$$\hat{D}f(x) = \lambda f(x), \quad (71)$$

where  $\lambda$  is a constant. As we know, there will be two independent solutions for this equation for each value of  $\lambda$ . Let us now impose some vanishing boundary conditions, say of Dirichlet type, which require  $f(x_a) = f(x_b) = 0$ . That is, in this case we are looking for modes. In general there will be no combination of the two independent solutions that can achieve these conditions, except for a discrete set of values of  $\lambda$ :

$$\hat{D}f_n(x) = \lambda_n f_n(x). \quad (72)$$

The functions  $f_n$  are called the eigenfunctions of the operator, and  $\lambda_n$  are the corresponding eigenvalues.

Without loss of generality, we can write this in terms of self-adjoint operators. By letting  $f_n = wu_n$  where  $w$  is the Wronskian, the eigenvalue equation becomes

$$\hat{D}u_n(x) = \lambda_n w(x)u_n(x). \quad (73)$$

Notice that the Wronskian  $w(x)$  plays the role of a weight function. As we discussed earlier, if  $p$ , the coefficient of the first derivative, is real and well behaved, then the Wronskian can be chosen to be always positive. The advantage of expressing this problem in terms of self-adjoint operators is that the eigenvalues and eigenfunctions can then be shown to

have several properties that are important in the study of waveguides and also in quantum mechanics. Consider the inner product of  $u_{n'}$  and both sides of Eq. (73):

$$\langle u_{n'}, \hat{\mathcal{D}}u_n \rangle = \langle u_{n'}, \lambda_n w u_n \rangle = \lambda_n \langle u_{n'}, u_n \rangle_w, \quad (74)$$

where we define the weighted inner product as

$$\langle v, u \rangle_w = \int_{x_a}^{x_b} v^*(x)u(x)w(x)dx. \quad (75)$$

However, we can use the defining property of a self-adjoint operator on the left-hand side of Eq. (74) which gives

$$\langle u_{n'}, \hat{\mathcal{D}}u_n \rangle = \langle \hat{\mathcal{D}}u_{n'}, u_n \rangle = \lambda_{n'}^* \langle u_{n'}, u_n \rangle_w. \quad (76)$$

Combining Eqs. (74) and (76), we can write

$$(\lambda_n - \lambda_{n'}^*) \langle u_{n'}, u_n \rangle_w = 0. \quad (77)$$

This equation has several consequences. First, notice that, because  $w(x) > 0$ , the inner product in Eq. (77) is positive when  $n = n'$ . Therefore, in this case, we get  $\lambda_n = \lambda_n^*$ , that is, all eigenvalues are real. If we choose  $n \neq n'$  and  $\lambda_n \neq \lambda_{n'}$ , then we find that the eigenfunctions are orthonormal:

$$\langle u_{n'}, u_n \rangle_w = 0. \quad (78)$$

In terms of the original functions  $f_n$ , this can be written as

$$\int_{x_a}^{x_b} f_{n'}^*(x)f_n(x)\frac{1}{w(x)}dx = 0. \quad (79)$$

Finally, if  $n \neq n'$  but it happens that  $\lambda_n = \lambda_{n'}$ , then we have what is called degeneracy, and we cannot be sure that  $\langle u_{n'}, u_n \rangle_w$  vanishes. However, by using an orthogonalization process, these functions can be redefined to be orthogonal.

As an exercise, find the orthogonality expression for the solutions of the Bessel equation.

Finally, the last important property follows from rewriting the eigenvalue equation in the explicit form

$$\hat{\mathcal{D}}u_n - \lambda_n u_n = [w(x)u_n'(x)]' + [\beta(x) - \lambda_n w(x)]u_n(x) = 0. \quad (80)$$

By using the results of Section IVA, it is easy to see that there are no eigenfunctions (modes) if

$$w(x)[\beta(x) - \lambda_n w(x)] < 0, \quad x \in [x_a, x_b]. \quad (81)$$



Because  $w(x) > 0$ , this means that there are no eigenfunctions when

$$\lambda_n w(x) > \beta(x), \quad x \in [x_a, x_b]. \quad (82)$$

This inequality places an upper bound on the eigenvalues  $\lambda_n$ . In other words, there is a possible maximum eigenvalue  $\lambda_0$ , which is greater or equal to all others. In quantum mechanics, the eigenfunction associated to this eigenvalue is called the ground state. In waveguides, this eigenfunction corresponds to the fundamental mode.

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- [1] G.B. Arfken and H.J. Weber, *Mathematical Methods for Physics*, 5th ed. (Harcourt Academic Press, San Diego, 2001).

These are the coefficients:

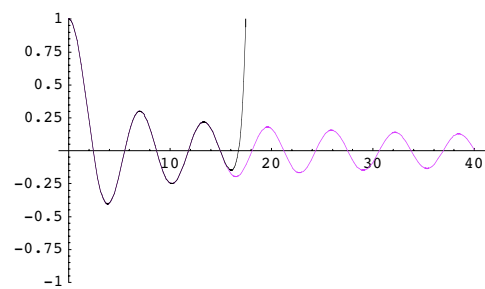
```
In[1]:= a[n_, v_] := If[Round[n/2] == n/2, If[n == 0, 1, -a[n-2, v] / (n (n + 2 v))], 0]
```

Here we sum the series up to n=nmax:

```
In[2]:= J[x_, v_, nmax_] = Sum[a[n, v] x^n, {n, 0, nmax}];
```

Here we plot the partial series for nmax=40 compared to the inbuilt function in mathematica (in purple):

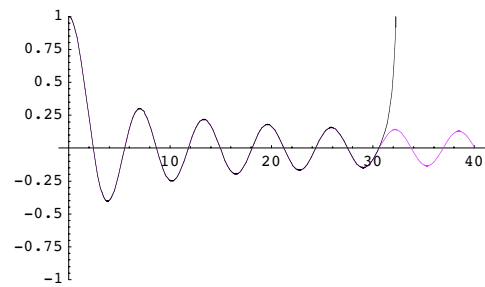
```
In[3]:= Plot[{BesselJ[0, x], J[x, 0, 40]}, {x, 0, 40}, PlotPoints -> 100,
  PlotRange -> {-1, 1}, PlotStyle -> {Hue[.8], GrayLevel[0]}]
```



Out[3]= - Graphics -

Here we plot the partial series for nmax=80 compared to the inbuilt function in mathematica (in purple):

```
In[4]:= Plot[{BesselJ[0, x], J[x, 0, 80]}, {x, 0, 40}, PlotPoints -> 100,
  PlotRange -> {-1, 1}, PlotStyle -> {Hue[.8], GrayLevel[0]}]
```



Out[4]= - Graphics -