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Neumann Functions and Its Application for Finding the Solution to the Schrödinger's Equation in a Cylindrical Well

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Abstract: Bessel Functions are series of solution to second order differential equation that arise in many diverse situations. This paper derives the Bessel functions through use of a series solution to differential equation, develops the different kinds of Bessel functions, and explores the topic of zeroes. Finally, Bessel functions are found to be the solution to the Schrödinger's equations in situation with cylindrical symmetry.

Keywords: Neumann functions, Modified Bessel Function, Modulation index, Cylindrical Well, Boundary Conditions

I. INTRODUCTION

This The boundary value problem (one dimensional heat equation) with cylindrical symmetry reduces to two ordinary differential equations by the separation of variable method. One of them is the most useful differential equation known as Bessel's differential equation.

equation was studied by Bessel with his work on planetary motion. Outside of planetary motion, the equation appears prominently in a wide range of applications such as steady and unsteady diffusion in cylindrical regions and one dimensional wave propagation etc. The subject of Bessel function and application is a very rich subject: nevertheless, due to space and time restrictions and interest of studying applications, the Bessel function shall be represented as a series solution to the second order differential equation, and then applied to a situation with cylindrical symmetry. Approximate development of zeroes, modified Bessel function and the application of boundary conditions will be briefly discussed.

II. NOTATIONS AND DEFINITIONS

An important differential equation which arises in mathematical physics is the Bessel equation

$$x^2 y'' + xy' + (x^2 - v^2)y = 0 \quad (1)$$

Where v is a constant

$$x(xy')' + (x^2 - v^2)y = 0 \quad (2)$$

And employing the use of Frobenius method, we re-write the terms of (2) in the terms of the series:

$$y = \sum_{n=0}^{\infty} a_n x^{n+s}$$

$$y' = \sum_{n=0}^{\infty} a_n (n+s) x^{n+s-1}$$

$$xy' = \sum_{n=0}^{\infty} a_n (n+s) x^{n+s}$$

$$(xy')' = \sum_{n=0}^{\infty} a_n (n+s)^2 x^{n+s-1}$$

When the coefficients of the powers of x are organized, we find that coefficient on x^s gives the indicial equation $s^2 - v^2 = 0, \Rightarrow s = \pm v$, we develop the general formula for the coefficient on the x^{s+n} terms:

$$a_n = -\frac{a_{n-2}}{(n+s)^2 - v^2} \quad (3)$$

In the case $s = v$

$$a_n = -\frac{a_{n-2}}{n(n+2v)} \quad (4)$$

And since $a_1 = 0$, $a_n = 0$ for all $n = \text{odd integers}$. Coefficients for even powers of n are found:

$$a_{2n} = -\frac{a_{2n-2}}{2^2 n(n+v)} \quad (5)$$

We can write the coefficient:

$$a_2 = -\frac{a_0}{2^{2(1+v)}} = -\frac{\Gamma(1+v)}{2^2 \Gamma(2+v)}$$

$$a_{2n} = -\frac{a_0 \Gamma(1+v)}{n! 2^{2n} \Gamma(n+1+v)}$$

This allows us to write the terms of the series:

$$y = J_v(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{\Gamma(n+1)\Gamma(n+1+v)} \left(\frac{x}{2}\right)^{2n+v} \quad (6)$$

Where $J_v(x)$ is the Bessel function of the first kind of order v .

Bessel function of the second kind is known as Neumann functions, are developed as a linear combination of Bessel function of the first order described:

$$N_v(x) = \frac{\cos v \pi J_v(x) - J_{-v}(x)}{\sin v \pi} \quad (7)$$

For integral values of v , the expression of $N_v(x)$ have a indeterminate form, and $N_v(x)|_{x=0} = \pm\infty$ nevertheless the limit of this function for $x \neq 0$, the expression for N_v is valid for any value of v , allowing the general solution to Bessel's equation to be written:

$$y = AJ_v(x) + BN_v(x) \quad (8)$$

With A and Barbitrary constants determined from boundary conditions

Bessel functions of the first and second kind are the most commonly found forms of the Bessel function in applications. Many applications in hydrodynamics, pumps, turbines, hydropower, modulated radio transmission, elasticity, and oscillatory systems have solutions that are based on the Bessel functions. One such example is that of a uniform density chain fixed at one end undergoing small oscillations. The differential equation of this situation is:

$$\frac{d^2 u}{dz^2} + \frac{1}{z} \frac{du}{dz} + \frac{k^2 u}{z} = 0 \quad (9)$$

Where z refers to a point on the chain, $k^2 = \frac{p^2}{g}$, with p as the frequency of small oscillation at that point, and g the gravitational constant of acceleration. Eq. (9) is a form of eq. (1), and solution is:

$$u = AJ_0\left(2kz^{\frac{1}{2}}\right) + BY_0\left(2kz^{\frac{1}{2}}\right), \quad (10)$$

Where A and B are determined by the boundary conditions.

Modified Bessel functions are found as solution to the modified Bessel equation

$$x^2 y'' + xy' - (x^2 - v^2)y = 0 \quad (11)$$

Which transforms into eq. (1) when x is replaced with ix . However; this leaves the general solution of eq. (1) a complex function of x . To avoid dealing with complex solutions in the practical applications, the solutions to (11) are expressed in the form:

$$I_v(x) = e^{\frac{v\pi i}{2}} J_v\left(xe^{\frac{i\pi}{2}}\right) \quad (12)$$

The $I_v(x)$ are set of functions known as the modified Bessel functions of the first kind. The general solutions of the modified Bessel function is expressed as a combination of $I_v(x)$ and a function $I_{-v}(x)$

$$y = AI_{-v}(x) - BI_v(x) \quad (13)$$

Where again A and B are determined from the boundary conditions.

A solution for non-integer orders of v is found:

$$K_v(x) = \frac{\pi I_{-v}(x) - I_v(x)}{2 \sin v \pi} \quad (14)$$

The functions $K_v(x)$ are known as modified Bessel functions of the second kind. Modified Bessel functions appears less frequently in applications, but can be found in transmission line studies, non-uniform beams, and the statistical treatment of a relativistic gas in statistical machines.

Bessel functions of the first and second kind have an infinite number of zeroes as the value of x goes to ∞

The modified Bessel function of the first kind ($I_\nu(x)$) have only one zero at the point $x = 0$, and the modified Bessel equation of the second kind ($K_\nu(x)$) functions do not have zeroes.

Bessel function zeroes are exploited in frequency modulated (FM) radio transmission. FM transmission is mathematically represented by a harmonic distribution of sine wave carrier modulated by a sine wave signal which can be represented with Bessel Functions. The carried frequencies disappear when the modulation index (the peak frequency deviation divided by the modulation frequency) is equal to the zero crossing of the function for the n^{th} sideband.

III. SOLUTION OF SCHRÖDINGER'S EQUATION IN A CYLINDRICAL WELL

Consider a particle of mass m placed into a two dimensional potential well, where the potential is zero inside the radius of the disk, infinite outside of the radius of the disk. In the polar coordinates using r, ϕ as representatives of the system, the Laplacian is written:

$$\Delta^2 \Psi = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \phi^2} \quad (15)$$

This in the Schrödinger equation presents:

$$-\frac{\hbar^2}{2m} \left[\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \Psi}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 \Psi}{\partial \phi^2} \right] = E \Psi \quad (16)$$

Using the method of separation of the variable with a proposed solution $\Psi = R(r)T(\phi)$ in (16), produces

$$-\frac{\hbar^2}{2m} \left[T(\phi) \frac{1}{R(r)} \frac{\partial}{\partial r} \left(r \frac{\partial R(r)}{\partial r} \right) + \frac{1}{r^2} R(r) \frac{\partial^2 T}{\partial \phi^2} \right] = ER(r)T(\phi) \quad (17)$$

and then dividing by Ψ :

$$\left[\frac{1}{R} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial R}{\partial r} \right) + \frac{1}{r^2} \frac{1}{T} \frac{\partial^2 T}{\partial \phi^2} \right] = \frac{-2mE}{\hbar^2} \quad (18)$$

setting $\frac{2mE}{\hbar^2} = k^2$ and multiplying by r^2 produces

$$\frac{r}{R} \frac{d}{dr} \left(r \frac{dR}{dr} \right) + k^2 r^2 + \frac{1}{T} \frac{d^2 T}{d\phi^2} = 0 \quad (19)$$

Which is fully separated in r and ϕ . To solve, the ϕ dependent portion is set to $-m^2$, yielding the harmonic oscillator equation in $T(\phi)$, which presents the solution:

$$T(\phi) = Ae^{im\phi} \quad (20)$$

Where A is a constant determined via proper normalization in ϕ :

$$\int_0^{2\pi} A^2 T(\phi) T(\phi) d\phi = 1 \Rightarrow A = \sqrt{\frac{1}{2\pi}} \quad (21)$$

Leaving the ϕ dependent portion $T(\phi) = \sqrt{\frac{1}{2\pi}} e^{im\phi}$

Work now with the r dependent portion of the separated equation, multiplying the r dependent portion of (19) by r^2 , and setting equal to m^2 one obtains:

$$\frac{r^2}{R} \frac{d^2 R}{dr^2} + \frac{r}{R} \frac{dR}{dr} + k^2 r^2 = m^2 \quad (22)$$

Which when rearranged:

$$r^2 \frac{d^2 R}{dr^2} + r \frac{dR}{dr} + (k^2 r^2 - m^2) R = 0 \quad (23)$$

This is one the same form as Eq. (1), Bessel differential equation. The general solution to Eq. (23) is the form of Eq. (8), and we write that general solution:

$$R(r) = AJ_m(kr) + BN_m(kr), \quad (24)$$

Where $J_m(kr)$ and $N_m(kr)$ are respectively the Bessel and Neumann function of order m , and A and B are constants to be determined via application of the boundary conditions. As the solution must be finite at $x = 0$ and as $N_m(kr) \rightarrow \infty$ as $x \rightarrow 0$, this means that the coefficient of $N_m(kr) = B = 0$, leaving $R(r)$ to be expressed:

$$R(r) = AJ_m(kr) \quad (25)$$

Using the boundary conditions $\Psi = 0$ at the radius of the disk, we have the condition that $J_m(kr_b) = 0$, which implicitly requires the argument J_m to be a zero of the Bessel function. As noted earlier, these zeroes must be so that $kr_b = \alpha_{m,n}$, which is the n^{th} zero of the m^{th} order Bessel function the energy system is solved by expressing k in terms of $\alpha_{m,n}$ in

(eq. $k = \sqrt{\frac{2mE}{\hbar^2}}$), arriving at:

$$E_{m,n} = \frac{\alpha_{m,n}^2 \hbar^2}{2mr_b^2} \quad (26)$$

The full solution for Ψ is thus:

$$\Psi_m(r, \phi) = AJ_m\left(\frac{\alpha_{m,n}r}{r_b}\right)e^{im\phi} \quad (27)$$

Because the Bessel function zeroes cannot be determined apriori, it is difficult to find a closed situation to express the normalization constant A. We select an order for m to continue with the determination of the normalization constant, and arbitrarily choose $m = 2$, which has a zero at $r = 5.13562$, which we will set to be the radius of the circle. Given the preceding, the normalization can be for $m = 2, n = 1$ case can be found:

$$\int_0^{r_{boundary}} A^2 J_2\left(\frac{\alpha_{2,1}r}{r_b}\right) J_2\left(\frac{\alpha_{2,1}r}{r_b}\right) dr = 1 \quad (28)$$

$$\text{Which for } r_{boundary} = 5.13562 \Rightarrow A = \sqrt{\frac{1}{0.510337}},$$

(Numerical values obtained using numerical integration). Thus we can express the full solution for $m = 2$ scenario:

$$\Psi(r, \phi) = \sqrt{\frac{1}{0.51377}} \sqrt{\frac{1}{2\pi}} J_2\left(\frac{\alpha_{2,1}r}{r_b}\right) e^{im\phi} \quad (29)$$

And since we have effectively set $\alpha_{m,n} = r_b$,

$$\Psi(r, \phi) = \sqrt{\frac{1}{0.51377}} \sqrt{\frac{1}{2\pi}} J_2(r) e^{im\phi} \quad (30)$$

Admittedly, this solution is somewhat contrived, but it shows the importance of working with the zeroes of the Bessel function to generate the particular solution using the boundary conditions.

IV. CONCLUSIONS

The Bessel function appears in many diverse scenarios, particularly situations involving cylindrical symmetry. The most difficult aspect of working with the Bessel functions is first, determining that they can be applied through reductions of the system equation to Bessel's differential or modified equation, and then manipulating boundary conditions with appropriate applications of zeroes, and the coefficient values in the augment of the Bessel function.

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