LECTURE 11 7-10-09

GENERAL SOLUTION

CARTESIAN

$$V(x,y,z) \sim e^{\pm i\alpha x} \, e^{\pm i\beta y} \, e^{\pm \gamma z}$$

SPHERICAL (AXIAL SYMMETRY)

$$V(r,\theta) = \sum_{\ell=0}^{\infty} \left[A_\ell r^\ell + B_\ell \frac{1}{r^{\ell+1}} \right] P_\ell(\cos\theta)$$

LEGENDRE POLYNOMIALS

SPHERICAL (WO AXIAL SYMMETRY)

$$V(r,\theta,\varphi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \left[A_\ell r^\ell + B_\ell \frac{1}{r^{\ell+1}} \right] Y_{\ell m}(\theta,\varphi)$$

SPHERICAL HARMONICS

CYLINDRICAL (W CYLINDRICAL SYMMETRY)

$$V(r,\theta) = A_0 + B_0 \ln r + \sum_{m=1}^{\infty} \left[A_m r^m + B_m \frac{1}{r^m} \right] \left[C_m \cos(m\theta) + D_m \sin(m\theta) \right]$$

CYLINDRICAL HARMONICS

CYLINDRICAL (NO CYLINDRICAL SYMMETRY)

$$V(r,\theta,z) \sim \sum_{\substack{m \\ n}} \left[A_{mn} J_n(k_m r) + B_{mn} N_n(k_m r) \right]$$

$$e^{\pm i n\theta} \quad e^{\pm k_m (z)}$$

J_n N_n CYLINDRICAL BESSEL FCNS

Spherical Coordinates

SPHERICAL COORDINATES

$$\nabla^2\Phi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\Phi}{\partial\varphi^2} = 0$$

$$\Phi(r,\theta,\varphi) = R(r)P(\theta)Q(\varphi)$$

$$\frac{1}{r^2 R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{1}{r^2 P\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \frac{1}{r^2 Q\sin^2\theta}\frac{d^2Q}{d\varphi^2} = 0$$

multiply with $r^2\sin^2\theta$:

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{P}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) = -\frac{1}{Q}\frac{d^2Q}{d\varphi^2}$$

The left-hand side depends only on r and θ, while the right-hand side depends only on ϕ. Thus the two sides must be a constant, m^2.

$$\frac{d^2Q}{d\varphi^2} + m^2 Q = 0 \quad ; \quad Q(\varphi) \sim e^{\pm im\varphi} \quad ; \quad m = 0,1,2\ldots$$

Note: If the physical problem limits ϕ to a restricted range m can be a non-integer.

Now we return to the left-hand side and rearrange the terms:

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) = -\frac{1}{P\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) + \frac{m^2}{\sin^2\theta}$$

The new left-hand side depends only on r and the right-hand side on only θ. Thus, they must be a constant, $l(l+1)$.

We get

$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - l(l+1)R = 0$$

and

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{dP}{d\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]P = 0$$

To solve the first, we make the ansatz: $R = Ar^{\alpha}$ and obtain the two solutions r^{l} and $r^{-(l+1)}$. The general solution is then

$$R_l(r) = A_l r^l + B_l \frac{1}{r^{l+1}}$$

For the polar-angle function $P(\theta)$ it is customary to make the substitution

$$\cos\theta \to x \quad ; \quad -\frac{1}{\sin\theta}\frac{d}{d\theta} \to \frac{d}{dx}$$

This gives

$$\frac{d}{dx}\left[\left(1-x^2\right)\frac{dP}{dx}\right] + \left[l(l+1) - \frac{m^2}{1-x^2}\right]P = 0$$

We will first limit ourselves to axial or azimuthal symmetry.

Axial symmetry

$$\boxed{\left(1-x^2\right)\frac{d^2P}{dx^2}-2x\frac{dP}{dx}+l(l+1)P=0}$$ *Legendre's equation*

Note that if $x=\pm 1$ are excluded from the problem l may be non-integer.

The solution is the *Legendre polynomial* of order l: $P_l(\cos\theta)$

Thus we have the general solution to Laplace's equation in spherical coordinates for the special case of axial symmetry as:

$$\boxed{\Phi(r,\theta)=\sum_{l=0}^{\infty}\left[A_l r^l+B_l\frac{1}{r^{l+1}}\right]P_l(\cos\theta)}$$

The Legendre polynomials can be obtained from

$$\boxed{P_l(x)=\frac{1}{2^l l!}\frac{d^l}{dx^l}\left(x^2-1\right)^l}$$ *Rodrigues' formula*

or from the *generating function*

$$F(x,\mu)=\frac{1}{\left(1-2x\mu+\mu^2\right)^{1/2}}=\sum_{l=0}^{\infty}\mu^l P_l(x)$$

or from *recursion relations* such as:

$$(l+1)P_{l+1}(x)=(2l+1)xP_l(x)-lP_{l-1}(x)$$

or

$$\left(1-x^2\right)\frac{dP_l}{dx}=-lxP_l(x)+lP_{l-1}(x)$$

The polynomials form a *complete, orthogonal set* of functions in the domain -1≤x≤1 (0≤θ≤π)

$$f(x) = \sum_{l=0}^{\infty} A_l P_l(x)$$

$$A_l = \frac{2l+1}{2} \int_{-1}^{1} f(x) P_l(x) dx$$

University of Nebraska
Department of Physics and Astronomy

Polarized Electron Physics

News

Pssst...Hey Mister...Wanna See a Picture of a Hexacontatetrapole?

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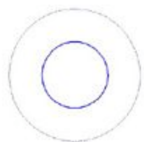
So what *is* a hexacontatetrapole moment, anyway?

A sum of sines and cosines can be used to model period functions, given the correct coefficients (a Fourier series). Similarly, a special set of polynomials known as Legendres can model functions in a spherical coordinate system: specifically, spherical harmonics. In our lab, we care about spherical harmonics when we're talking about atomic orbitals--these charge clouds can be modeled using a series of Legendres. The collection of necessary parameters are known as the multipole moments.

Multipoles have many uses throughout the physical sciences. One common example comes from computational chemistry: predicting the electric potential (voltage) field due to a complex molecule. You could find the components of the field at each point due to every atom, but this becomes a tremendous task with a large molecule. Instead, the molecule can be decomposed into a handful of multipole moments which provide simple equations for predicting the field.

In essence, multipoles describe how much something behaves like another system that we can predict easily.



We start by asking, "How much does this act like a ball of charge?" In that case, the potential field is distributed evenly in all directions, and our multipole moment is an estimate of the total charge.

Next, we ask about how much the field behaves like a dipole: two opposite charges seperated by a small distance. In this case, the field has two bulbous ends, one with a positive potential and the other with negative potential. This multipole moment is something like the center of charge, giving us a clue to the distance between our origin and the center of charge. In some sense, the dipole is similar to the center of mass for a solid object.

As more charges are arranged together, they start creating strange looking fields. The beauty of the mathematics is that all the fields fit together to create a more complete picture of the field. We have information about the charge and center of mass from the first two poles, then keep adding finer and finer details until we have an adequate idea of the field's behavior. In the case of our hexacontatetrapole, that's seven poles deep, and we have an excellent measurement of how the system is behaving.

In an experiment, we start with data, extract multipoles, and try to reassemble the original field. Depending on the mathematics, this can give a single field solution or a set of solutions. While we can go backwards in some cases, the important information is not necessarily the original field, but how that field behaves. This is again where the multipoles come in handy: based on the multipole data, we can anticipate a reaction to the field without knowing what it true shape is, and we can gather hints about what the shape might be.

Let's take three examples, and look at what we can predict about the fields based on the multipoles. We'll use a football, a discus, and a bowling pin as familiar examples with differing poles. Each has a well defined axis of rotation, but differ in their symmetries around an equatorial axis. The football is longer in the axial direction, whereas the discus is wider in the equatorial direction than it is long. The bowling pin is not symmetric about its equator, since one end bulges out much more than the other.

To calculate the multipoles, we took a photograph of each object, then plotted points along its outline to simulate data. Next, we used integration to fit multipoles to the data sets, similar to the experiments in our lab. Those values are listed in the following table:

Order	Name	Football	Discus	Bowling Pin
0	Monopole	1	1	1
1	Dipole	0	0	-3.15×10^{-2}
2	Quadrupole	2.35×10^{-3}	-4.13×10^{-3}	5.22×10^{-3}

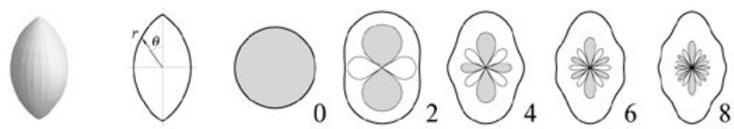
3	Octupole	0	0	-1.56×10^{-4}
		. . .		
6	Hexacontatetrapole	1.38×10^{-7}	-4.84×10^{-7}	6.61×10^{-7}

The first thing to notice is that if the object or field is symmetric, like the football and discus, all the odd-ordered multipoles are zero. These odd multipoles are all based on Legendre polynomials that are non-symmetric, so we wouldn't expect them in a symmetric object. Secondly, the sign of the multipole indicates whether there is an addition or subtraction from the field. The football has positive multipoles, and continues to grow slowly in the axial direction. The discus alternates sign, causing it to shrink a small amount more than it grows in the axial direction, making it wider in the equatorial direction.

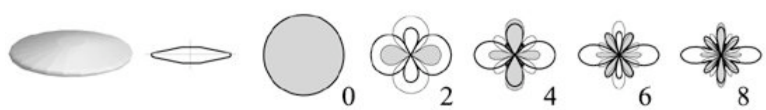
Great, we can calculate interactions. But what about the original field?

Multipoles can give us a good idea of how the field *behaves* without having to know the original field. In some cases, we can actually go backwards to create a field. For our sports balls, we can only generate one field of an infinite number of fields, but we'll see that given some guesses about the original size, our generalizations about what multipoles come from which shape will hold.

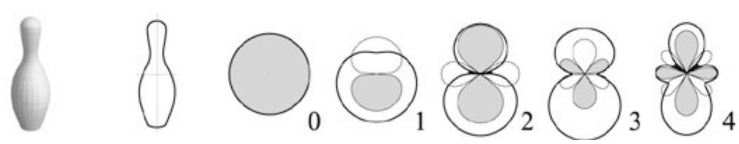
Again using multipoles, we can create spheres of varying density that yield pure multipole moments. A sphere with a density that varies in the same way as a dipole will end up with *only* a dipole momen, nothing else. By assembling these spheres together with the right weights, we create a new sphere that is composed of only pure multipole moments, and will thus yield the same multipoles.



Above is a reconstruction of the football, assuming a radius of 15 cm. The index is the highest order of multipoles used in that reconstruction, with zero being the monopole and six being the hexacontatetrapole. We've taken the mutipole spheres and graphed radius as a function of density; these are the thick black lines. Each additional multipole is shown in grey and white, where grey is an addition and white is a subtraction. These illustrate how the multipoles influence the overall shape. With the football, the "shape", or the thick black line, becomes longer in the axial direction, and has the general shape of a football.



The discus is quite a bit different from the football. It gets shorter in the axial direction and slowly grows in the equatorial direction. The shape line is complex, so it's hard to say that at this order we've got a discus, but many of the characteristics are the same. Note that this shape gives the same multipoles as the discus we are familiar with. In this reconstruction, the bulbous ends of the multipoles along the axis alternate positive and negative, just as the multipole moments did. However, there is always a grey positive addition along the equatorial plane.



The bowling pin is unique in that it has both odd and even multipoles. As the reconstruction progresses, the bottom end becomes larger and the top end becomes slightly smaller. The neck region shrinks, and the net shape resembles the beginnings of a bowling pin. The multipoles have signs such that the grey positive addition is towards the bulbous end.

These examples illustrate that you can get a general sense of the original field based on the multipoles, but (depending on the mathematics) the original field may not be reconstructable.

So, what is a hexacontatetrapole?

Despite the long name, it's just the 7th layer (6th order) of detail for a system represented by multipoles. It gives another level of information for understanding exactly what's going on in an interaction. In the end, we even have a better idea of what the charge cloud looks like in the system under study.

For our lab, and many other areas of physical science, multipoles are useful tools.

General case, no axial symmetry.

In this case we have in general a non-zero m value and the differential equation for P is more elaborate. The Legendre polynomials are replaced by the *associated Legendre polynomials*, $P_l^m(\cos\theta)$. For a given l-value there are $2l$+1 possible m-values: m = 0, ±1, ±2,, ±3, ...

There is a more general *Rodrigues' formula* for these functions:

$$P_l^m(x) = \frac{(-1)^m}{2^l\, l!}\left(1 - x^2\right)^{m/2} \frac{d^{l+m}}{dx^{l+m}}\left(x^2 - 1\right)^l \quad ; \quad (-l \le m \le +l)$$

For any given m the functions $P_l^m(\cos\theta)$ and $P_{l'}^m(\cos\theta)$ are orthogonal and the associated Legendre polynomials for a fixed m form a complete set of functions in the variable x.

The product of $P_l^m(x)$ and $e^{im\varphi}$ forms a complete set for the expansion of an arbitrary function on the surface of a sphere. These functions are called *spherical harmonics*.

$$\boxed{Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta) e^{im\varphi}}$$

They are orthonormal

$$\begin{aligned} &\int_{4\pi} Y_l^m(\theta,\varphi) Y_{l'}^{m'} * (\theta,\varphi) d\Omega \\ &\quad = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin\theta d\theta Y_l^m(\theta,\varphi) Y_{l'}^{m'} * (\theta,\varphi) = \delta_{ll'}\delta_{mm'} \end{aligned}$$

$$f(\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} C_l^m Y_l^m(\theta,\varphi)$$

and

$$C_l^m = \int_{4\pi} f(\theta,\varphi) Y_l^m * (\theta,\varphi) d\Omega$$

The general solution to Laplace's equation in terms of spherical harmonics is

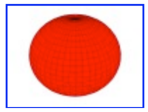
$$\boxed{\Phi(r,\theta,\varphi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}\left[A_l^m r^l + B_l^m \frac{1}{r^{l+1}}\right] Y_l^m(\theta,\varphi)}$$

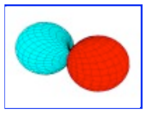
Spherical Harmonics

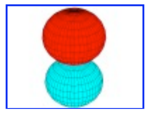
The Spherical Harmonics, $Y_{\ell,m}(\theta, \phi)$, are functions defined on the sphere. They are used to describe the wave function of the electron in a hydrogen atom, oscillations of a soap bubble, etc. The spherical harmonics describe non-symmetric solutions to problems with spherical symmetry.

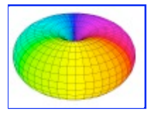
The $Y_{\ell,m}$'s are complex valued. The radius of the figure is the magnitude, and the color shows the phase, of $Y_{\ell,m}(\theta, \phi)$. These are the numbers on the unit circle: 1 is red, i is purple, -1 is cyan (light blue), and -i is yellow-green.

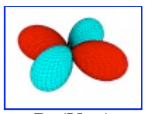
For each value of ℓ, there are $2\ell + 1$ linearly independent functions $Y_{\ell,m}$, where $m = -\ell, -\ell+1, \ldots, \ell-1, \ell$. I have chosen a different set of $2\ell + 1$ functions, as you see below.

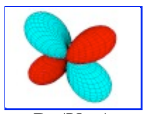

$Y_{0,0}$

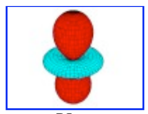

$\mathrm{Re}(Y_{1,1})$

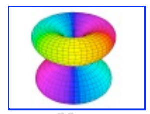

$Y_{1,0}$

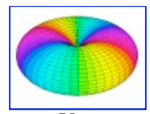

$Y_{1,1}$


$\mathrm{Re}(Y_{2,2})$


$\mathrm{Re}(Y_{2,1})$


$Y_{2,0}$

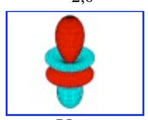

$Y_{2,1}$

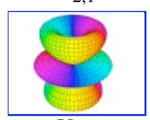

$Y_{2,2}$

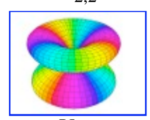

$\mathrm{Re}(Y_{3,3})$

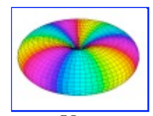

$\mathrm{Re}(Y_{3,2})$


$\mathrm{Re}(Y_{3,1})$

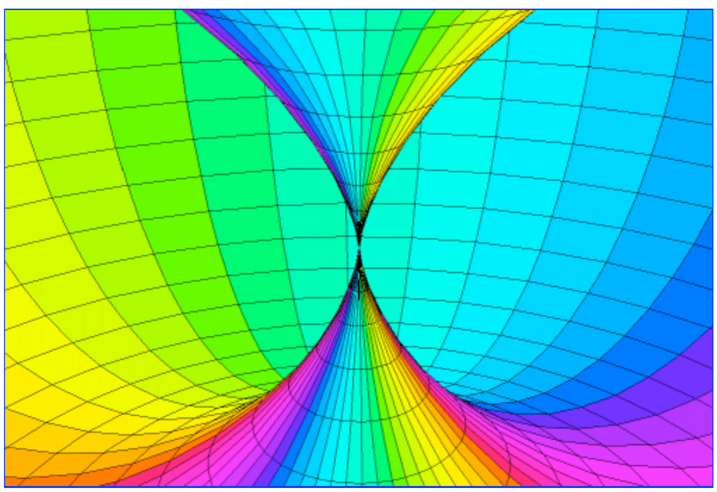

$Y_{3,0}$


$Y_{3,1}$


$Y_{3,2}$


$Y_{3,3}$

The following figure is called "inside $Y_{2,2}$". My son, Michael, made this by holding down the "Page Up" key until the viewpoint gets *inside* the surface. (He suggests that you set the figure rotating continuously, and move the viewpoint a bit down before zooming in.)



Oscillations of a Soap Bubble
The volume of the bubble is constant, so $Y_{0,0}$ is not used. The center of mass of the bubble is constant, so $Y_{1,m}$ is not used. The lowest frequency oscillations of a soap bubble are $\ell = 2$. The radius of the soap film is $r = 1 + \varepsilon\, Y_{2,m}(\theta, \phi)$. The oscillations with different m all have the same frequency. The shape of the oscillations with m = 1 and m = 2 are the same up to a rotation, but the m = 0 oscillation is different.

Physics and Math notation
WARNING: Spherical coordinates are different in physics and mathematics. The symbols θ and ϕ are switched! The math notation makes r and θ the same in cylincrical and spherical coordinates. DPGraph uses math notation.

$$x^2 + y^2 + z^2 = r^2 \text{ (physics)} = r^2 \text{ (math)}$$
$$\arccos(z/r) = \theta \text{ (physics)} = \phi \text{ (math)}$$

Cylindrical Coordinates

CYLINDRICAL COORDINATES

$$\nabla^2\Phi = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2\Phi}{\partial\theta^2} + \frac{\partial^2\Phi}{\partial z^2} = 0$$

$$\Phi(r,\theta,z) = R(r)Q(\theta)Z(z)$$

$$\frac{1}{rR(r)}\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right) + \frac{1}{r^2Q(\theta)}\frac{d^2Q(\theta)}{d\theta^2} + \frac{1}{Z(z)}\frac{d^2Z(z)}{dz^2} = 0$$

$$\frac{r}{R(r)}\frac{d}{dr}\left(r\frac{dR(r)}{dr}\right) + \frac{r^2}{Z(z)}\frac{d^2Z(z)}{dz^2} = -\frac{1}{Q(\theta)}\frac{d^2Q(\theta)}{d\theta^2} = n^2$$

$$\frac{d^2Q}{d\theta^2} + n^2Q = 0$$

$Q(\theta) \sim e^{\pm in\theta}$; $n = 0,1,2,\ldots$ (n may sometimes be non-integer)

$$\frac{1}{rR}\frac{d}{dr}\left(r\frac{dR}{dr}\right) - \frac{n^2}{r^2} = -\frac{1}{Z}\frac{d^2Z}{dz^2} = -k^2$$

$$\frac{d^2Z}{dz^2} - k^2Z = 0$$

$$Z(z) \sim e^{\pm kz}$$

$$r\frac{d}{dr}\left(r\frac{dR}{dr}\right) + \left(k^2r^2 - n^2\right)R = 0$$

Cylindrical symmetry and Cylindrical Harmonics

Then we may let k vanish and

$$r\frac{d}{dr}\left(r\frac{dR}{dr}\right) - n^2 R = 0$$

The n = 0 term has to be treated separately

$$R_n(r) = \begin{cases} A_0 + B_0 \ln r, \; (n=0) \\ A_n r^n + B_n \dfrac{1}{r^n}, \; (n = 1,2,3\ldots) \end{cases}$$

$$Q_n(\theta) = \begin{cases} C_0\left[+D_0\theta\right], \; (n=0) \\ C_n \cos n\theta + D_n \sin n\theta, \; (n = 1,2,3\ldots) \end{cases}$$

General solution in cylindrical coordinates with no z-dependence.

$$\boxed{\Phi(r,\theta) = A_0 + B_0 \ln r + \sum_{n=1}^{\infty}\left[A_n r^n + B_n \frac{1}{r^n}\right]\left[C_n \cos n\theta + D_n \sin n\theta\right]}$$

The terms are called *cylindrical harmonics*.

No cylindrical symmetry and Bessel functions.

Now, we have to keep the constant k in the differential equation for R.

$$r\frac{d}{dr}\left(r\frac{dR}{dr}\right)+\left(k^2r^2-n^2\right)R=0$$

To solve this one usually makes the substitution

$$u=kr\quad;\quad\frac{d}{dr}=k\frac{d}{du}$$

This leads to *Bessel's equation*:

$$\boxed{u^2\frac{d^2R}{du^2}+u\frac{dR}{du}+\left(u^2-n^2\right)R=0}$$

The solution to this equation is the so-called *Bessel function of order n*, $J_n(u)$. $J_{-n}(u)$ is also a solution. These are linearly dependent for integer orders but not for non-integer orders.

One usually introduces another function instead of $J_{-n}(u)$, the so-called *Neumann function* or *Bessel function of the second kind*, $N_n(u)$.

$$N_n(u)=\frac{J_n(u)\cos n\pi-J_{-n}(u)}{\sin n\pi}$$

General solution to Bessel's equation may be written as

$$R_n(kr)=A_nJ_n(kr)+B_nN_n(kr)$$

$J_n(u)$ is regular at origin and at infinity.
$N_n(u)$ is <u>not</u> regular at origin but at infinity.

The general solution to Laplace's equation in cylindrical coordinates can be written as the *Fourier-Bessel expansion*:

$$\boxed{\Phi(r,\theta,z) \sim \sum_{m,n}\left[A_{mn}J_n(k_m r) + B_{mn}N_n(k_m r)\right]e^{\pm in\theta}e^{\pm k_m z}}$$

Other useful properties of the Bessel function

Let $k_m\rho$ be the mth root of $J_n(kr)$, i.e., $J_n(k_m\rho) = 0$.

Then $J_n(k_m r)$ form a complete orthogonal set for the expansion of a function of r in the interval $0 \le r \le \rho$.

$$f(r) = \sum_{m=1}^{\infty} D_{mn}J_n(k_m r) \qquad (\text{for any } n)$$

Fourier-Bessel series

$$D_{mn} = \frac{2}{\rho^2 J_{n+1}^2(k_m\rho)}\int_0^{\infty} f(r)J_n(k_m r)rdr$$

analogous to the Fourier transform.

Discussion: If we had chosen $+k^2$ instead of $-k^2$:

$$\frac{1}{rR}\frac{d}{dr}\left(r\frac{dR}{dr}\right)-\frac{n^2}{r^2}=-\frac{1}{Z}\frac{d^2Z}{dz^2}=+k^2$$

The z- dependence had been plane waves instead of exponentials and the r dependence had been found as solutions to the *modified Bessel equation:*

$$\boxed{u^2\frac{d^2R}{du^2}+u\frac{dR}{du}-\left(u^2+n^2\right)R=0}$$

with the modified Bessel functions $I_n(u)$ and $K_n(u)$ as solutions. The first is bounded for small arguments and the second for large.

Thus, an alternative expression for the general solution is

$$\boxed{\Phi(r,\theta,z)\sim\sum_{m.n}\left[A_{mn}I_n\left(k_mr\right)+B_{mn}K_n\left(k_mr\right)\right]e^{\pm in\theta}e^{\pm ik_mz}}$$